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Structural phase stability, elastic parameters and thermal properties of YN from first-principles calculation

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Research Highlights

- The YN structural and elastic properties at normal and pressure are reported.
- The phase transition from the NaCl structure to the CsCl structure is addressed.
- The linear pressure coefficients of studied elastic moduli are also examined.
- The dynamical stability criteria and the phonon dispersion have been considered.
- The stability criteria are shown to be satisfied for YN under normal conditions.

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