

# T-USPEX method for constructing a nitrogen phase diagram under extreme conditions

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It is known that nitrogen at high P-T conditions is the first molecular system that passes into the polymer state before the metallization process [1]. The huge difference between the binding energy in polymer nitrogen ( $\sim 160$  kJ/mol) and a triple-bonded molecule ( $\sim 954$  kJ/mol) is responsible for large amount of energy that can be released during the transition from the polymer state to diatomic nitrogen connected by a triple bond [2]. In this way, one of the most attractive and promising areas for the application of such non-molecular nitrogen is the creation of high energy density materials (HEDM) [3]. Therefore, determination of the phase transition between nitrogen structures makes it possible to construct a phase diagram of nitrogen at high pressures and temperatures. In this work we determined the P-T stability regions of four known nitrogen phases: cg-N, LP-N, BP-N, HLP-N and construct a phase diagram at pressures from 120 to 250 GPa and temperatures from 1500 to 3500 K, using the algorithm T-USPEX.

- [1] Tomasino D, Kim M, Smith J and Yoo C S 2014 *Physical review letters* **113** 205502
- [2] Cheng P, Yang X, Zhang X, Wang Y, Jiang S and Goncharov A F 2020 *The Journal of Chemical Physics* **152** 244502
- [3] Ma Y, Oganov A R, Li Z, Xie Y and Kotakoski J 2009 *Physical Review Letters* **102** 065501