Bipentazole (N_{10}): A Low-Energy Molecular Nitrogen Allotrope with High Intrinsic Stability

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ABSTRACT: In this Letter, we report a crystal structure prediction and characterization of a molecular nitrogen allotrope N_{10} (bipentazole) using state-of-the-art computational methods. To date, in the form of a $P2_1$ space group crystal, this allotrope is the most stable predicted form of nitrogen, other than N_2, in the pressure range 0−42 GPa. Its metastability at ambient conditions was justified using phonon dispersion and mechanical properties calculations as well as *ab initio* molecular dynamics simulations. Due to a high intrinsic stability caused by aromaticity, bipentazole may appear to be the first nitrogen allotrope stable enough for a large-scale synthesis at ambient conditions. The calculations of propulsive characteristics revealed that bipentazole is an excellent "green" energetic material. A potential strategy for the synthesis of this compound is offered and rationalized. The unique electronic structure of bipentazole makes it a strongly electrophilic all-nitrogen reagent, which can exhibit unusual chemistry.

STRONGLY AROMATIC, ELECTROPHILIC AND ENERGETIC NITROGEN ALLOTROPE

BIPENTAZOLE
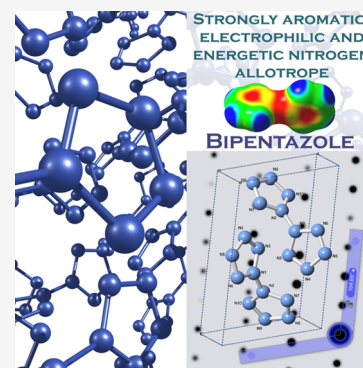
Recently, interest in nitrogen allotropes substantially increased, especially due to extension of the working pressure range in diamond anvil cell (DAC) experiments.[1−4] However, because of an extremely strong triple bond in a dinitrogen molecule (945 kJ mol^{-1}), the number of other experimentally obtained allotropes or compounds of polymeric nitrogen is just a few. Among these, one can find both polymeric (cg-N, $Pba2$, $P4_2bc$, $-(NH)_n-$, $-(Mg_xN_y)_n-$, $-(Fe_xN_y)_n-$, $ReN_8 \cdot xN_2$)[1−7] and molecular (N_8 and N_8^-)[8−10] forms. First-principles calculations, however, predict a much more extended set of the possible allotropes,[11−16] which probably can be accessible in the future (see our recent papers for more references).[17,18] The molecular form N_8 is the lowest energy allotrope in the low pressure range, which has recently been observed under 40 GPa, and its traces remained down to 3 GPa.[8] Furthermore, the cg-N allotrope has also recently been obtained at near ambient conditions.[19] These great discoveries inspired us to search more stable phases of nitrogen, which can be more easily obtained under ambient conditions.

Meanwhile, a great number of molecular and ionic forms of nitrogen (N_3^-, N_4, N_5^-, N_5^+, N_6, N_8, N_{10}, and N_{60}) was also calculated.[20,21] Among these molecular forms, an intriguing structure is bipentazole (N_{10}). Since its first mention in the literature in 1992,[22] this molecule has been ignored by researchers who work in the field of nitrogen allotropes, except for a couple of works.[23,24] However, due to the formation of strongly aromatic pentazole rings, bipentazole has significant gain in thermodynamic stability compared to the linear N_8 molecule. Our comparison of total energies of various molecular forms of nitrogen with the lower energy N_8 isomer EZE[10] is presented in Table S1 in the Supporting Information. It is clear that a bipentazole molecule is much more stable than EZE-N_8 ((Z)-1,2-diazidodiazene) by *ca.* 15 kJ mol^{-1} atom^{-1}. This means that bipentazole should be a more favorable molecular nitrogen allotrope from the thermodynamic point of view. Thus, we have performed an extensive crystal structure prediction and characterization of this possible allotrope, which is reported below.

Complete description of the computational procedures applied in this work along with the corresponding references is presented in the Supporting Information. As a result of this crystal structure prediction, we have found a set of possible structures, which are lower in energy than EZE-N_8 (Figure S1 in the Supporting Information), but only three of them, $P222$, $I222$, and $P2_1$, are dynamically and mechanically stable. The latter structure has the lowest enthalpy of formation and the highest cohesive energy (815.9 and 82.9 kJ mol^{-1}, respectively) and all further discussions will concern this allotrope (Figure 1a). Thus, the optimized asymmetric cell along with the molecular properties, crystal morphology, and dynamical and mechanical stability description is presented in Figure 1a−e. Crystal packing and fractional coordinates are listed in Figure S2 and Table S2 in the Supporting Information. Analogues description of the $I222$ and $P222$ allotropes can be found in Figures S3−S6 in the Supporting Information.
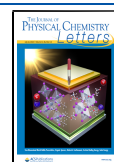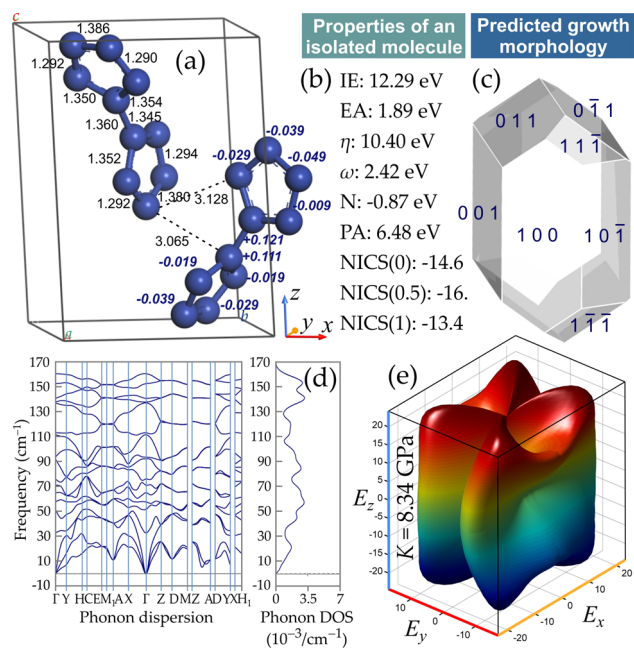
Figure 1. (a) Optimized asymmetric cell with structural parameters indicated [bond lengths in Å (regular values) and Hirshfeld charges in e^- (bold italic values)], (b) calculated molecular properties, (c) predicted vacuum growth morphology, (d) phonon dispersion and density of phonon states, and (e) 3D map of the Young modulus.

An isolated bipentaloze molecule exists in the D_{2d} point group symmetry. Meanwhile, in the crystalline state, the symmetry is completely broken; though, it is still close to the D_2 point group. The molecular properties in Figure 1b indicate a unique electronic structure of bipentazole (see Computational Details for descriptions). On one hand, despite the presence of lone pairs on the nitrogen atoms, N_{10} has extremely weak nucleophilic character, which is less than in tetracyanoethylene (TCE), a common reference with the lowest value ($N = 0$ eV).[25] On the other hand, electrophilicity of N_{10} is also less than in TCE ($\omega = 3.53$ eV) being intermediate among TCE, EZE-N_8 (1.64 eV), and NH_3 ($\omega = 1.04$ eV).[26] Thus, bipentazole can be considered as a strong electrophile[27] that approaches the electron-deficient 2,5-dinitro-1,4,2,3,5,6-dioxatetrazinane.[28] Despite its low nucleophilicity, N_{10} can be protonated, most likely in strong acidic media, which does not lead to the decomposition of the molecule.

The predicted crystal habit of bipentazole has seven stable faces (Figure 1c), whose Connolly surfaces are illustrated in Figure S7 in the Supporting Information. It is seen that all the surfaces are rather flat, except for (001) and (011). Thus, solvents, probably, do not have a significant impact on the growth morphology. Numerical parameters of the crystal habit are listed in Table S3 in the Supporting Information. As it follows from Figure 1d−e, bipentazole is dynamically and mechanically stable in the $P2_1$ space group. The calculated elastic stiffness and compliance constants are listed in Tables S4 and S5 in the Supporting Information. The bipentazole crystal has a bulk modulus that is typical for organic molecular crystals;[29] however, it possesses a strong anisotropy of the Young modulus (Figure 1e).

Apart from the dynamical and mechanical stability criteria, we have performed *ab initio* molecular dynamics simulations in order to check thermal stability of bipentazole at ambient temperature. Thus, we have performed a 10 ps simulation (time

step 1 fs) with *NVT* ensemble at 298 K. The supercell containing eight bipentazole units after the simulation is illustrated in Figure S8 in the Supporting Information. As one can see, all the bipentazole molecules appear to be thermally stable at ambient temperature.

To determine relative enthalpies of bipentazole and other nitrogen allotropes at different pressures, we have built the corresponding diagram, which is illustrated in Figure 2. For
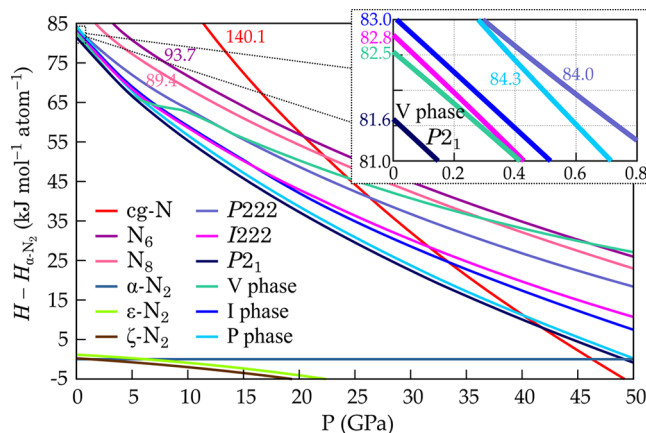

Figure 2. Enthalpies of several polymeric and molecular nitrogen allotropes at different pressures with respect to the enthalpy of α-N_2.

geometry optimization, we have applied step size 1 GPa (up to 5 GPa) and 5 GPa for the remaining pressure region. Remarkably, bipentazole has the lowest enthalpy in the pressure range 0−42 GPa. Any other nitrogen allotrope, including recently obtained molecular form N_8, is significantly higher in energy than bipentazole. It is interesting that the other two predicted forms of N_{10}, $I222$ and $P222$, are also always lower than N_8. Only above 42 GPa, the polymeric cubic *gauche* nitrogen allotrope cg-N becomes more stable than bipentazole (Figure 2). Thus, estimated enthalpies of formation of bipentazole and N_8 are 81.6 and 89.4 kJ mol^{-1} atom^{-1}, respectively.

In order to provide experimentalists with spectral data for further instrumental identification of bipentazole, we have calculated vibrational (infrared IR and Raman), electronic, and NMR spectra as well as X-ray diffraction pattern. A part of these data are illustrated in Figure 3 and all other spectral properties are gathered in Tables S6−S7 and Figures S9−S11 in the Supporting Information. The Raman spectrum demonstrates a very intense band at 1413 cm^{-1} (615 Å^4), which corresponds to the $\nu_{N1-N1'}$ valence vibration. Frequencies of all other valence vibrations (ν_{N2-N3} and ν_{N3-N4}) are in complete agreement with the predominant resonance structure of bipentazole possessing the N2−N3 double bonds (Figure 3a). In the calculated electronic spectrum (Figure 3b), the first band appears at about 200 nm. Thus, bipentazole is expected to be transparent solid. The predicted X-ray diffraction pattern and nature of the first eight electronic transitions are illustrated in Figure 3c,d.

The temperature dependence of the calculated thermodynamic properties of bipentazole (Figure S12) and enthalpy of formation were used to define a new reactant for the NASA CEA program (see the Supporting Information for details). Using these data, we have calculated propulsive properties of bipentazole as a solid monopropellant (Table S8 in the Supporting Information). As one can see, N_{10} demonstrates an excellent specific impulse ($I_{sp} = 295$ s) and characteristic velocity
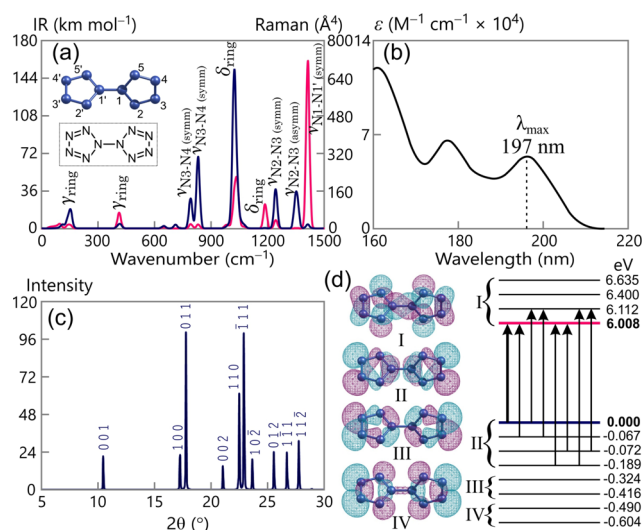
Figure 3. Calculated spectral properties of bipentazole.

($c^* = 1813$ m s^{-1}), which are significantly higher than that of most conventional energetic materials.

An important question arises: how can bipentazole be obtained experimentally? We speculate that the most probable way for obtaining this nitrogen allotrope is electrolysis of ammonium pentazolate salts.[30−33] Recently, a simple and versatile method for preparation of such salts was reported.[34,35] It is worth noting that the USPEX method applied in this work demonstrated success in prediction of the structure of such salts.[36−38]

Thus, our proposed strategy can be seen in Figure 4. Pentazolate anions and ammonium cations transform to the
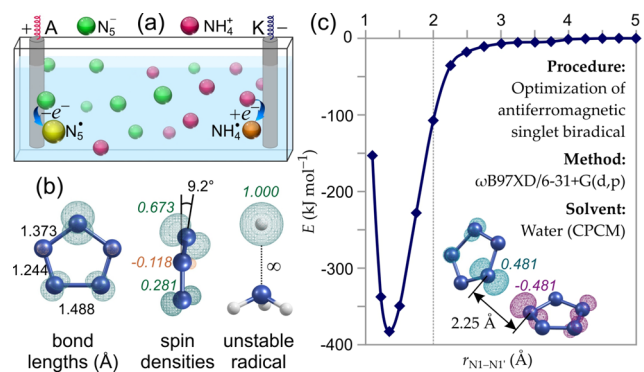

Figure 4. Proposed strategy for the synthesis of bipentazole.

corresponding radicals ($N_5^\bullet$ and $NH_4^\bullet$) on the surfaces of anode and cathode, respectively (Figure 4a). Recently, we have also predicted formation of such radical pairs in crystals of energetic salts undergone compression.[39] Pentazolyl radicals appeared to be stable in water medium, which follows from our PCM-DFT calculations. These possess the C_s symmetry with the N1 atom lying out of the ring plane by 9.2° (Figure 4b). This is a typical π-radical bearing main part of spin density on the 2p orbital of the N1 atom. We suppose that these radicals can recombine to form a bipentazole molecule.

This process is barrierless and strongly exothermic with the enthalpy of the reaction equal to −382.4 kJ mol^{-1} (Figure 4c). Using the procedure for antiferromagnetic coupling calculation, we have built appropriate initial guesses (with α and β spins on

each radical) and performed geometry optimizations and frequency calculations. As a result, the corresponding potential energy profile was built (Figure 4c). Up to a distance of 2.0 Å between the radicals, spin densities are absent, which indicates the unbroken N1−N1′ bond. At larger distances, the N1−N1′ bond is broken and nonzero spin densities appear. The numerical values of spin densities along with frequencies of the first vibration are listed in Table S9 and transformations of geometry along the potential energy profile are illustrated in Figure S13 in the Supporting Information.

Meanwhile, the formed $NH_4^\bullet$ radical is completely unstable and decomposes into an ammonia molecule and a hydrogen atom. We should stress that this reaction is characteristic for other ammonium-type cations ($HO-NH_3^+$, $NH_2-NH_3^+$, etc.). Thus, reactions of the formed radicals can be expressed as the following:

$$2\,NH_4^\bullet \longrightarrow 2\,NH_3 + H_2\uparrow$$
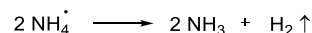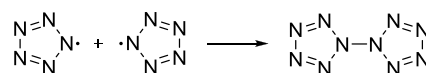
The newly formed molecules of ammonia further dissolve and dissociate into NH_4^+ and OH^- to give H_2 and O_2 on the cathode and anode, respectively.

In summary, we have reported a comprehensive study of a novel molecular nitrogen allotrope, bipentazole N_{10}. This molecule has the lowest enthalpy of any other nitrogen allotropes hitherto obtained experimentally or predicted theoretically, except for various forms of N_2. Only above 42 GPa does the cg-N allotrope become more stable than N_{10}. Bipentazole is dynamically, mechanically, and thermally stable under ambient conditions both in the crystalline state and polar media. Therefore, it is likely to be synthesized. We propose a synthetic route involving electrolysis of ammonium salts of the pentazolate anion; however, other methods may appear to be more successful.

If synthesized, bipentazole can find a number of possible practical applications in synthesis of energetic materials, propellants, etc. However, N_{10} may appear to be the first nitrogen allotrope that is stable enough for synthesis at macroscopic scale at ambient conditions.

■ ASSOCIATED CONTENT

ⓢ Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jpclett.0c01542.

> Energies of molecules N_x, computational details, crystal packing, fractional coordinates, stable crystal habit surfaces, elastic stiffness and compliance constants, supercell after molecular dynamics simulation, phonon dispersion, optimized geometries, eigenvectors of the vibrational modes, IR, Raman, NMR, optical, and propulsive properties, band structure and partial density of states, chemical shielding and EFG tensors, temperature dependence of thermodynamic properties, NASA coefficients, spin densities and transformations of geometry (PDF)

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Notes
The author declares no competing financial interest.
When the manuscript was completely ready for submission, another paper was published, in which bipentazole crystals are predicted.[40] The authors report a *P4/mbn* crystal to be stable at ambient conditions (the V phase). We have compared this crystal structure with our predicted *P2*$_1$ crystal and the latter still appeared to be more stable by 9.4 kJ mol^{-1}. The *P4/mbn* allotrope is a bit lower in energy than the *I222* structure (Figure 2). Starting from 10 GPa, the V phase demonstrates a flat region and after 15 GPa this becomes the highest-energy phase among all the N$_{10}$ crystals studied. At the same time, the P phase behaves similarly to the *P2*$_1$ allotrope but has a higher enthalpy for the entire pressure range up to 50 GPa (Figure 2). Moreover, according to our calculations, the *P4/mbn* crystal possesses dynamical as well as mechanical instability, which follows from the corresponding phonon dispersion and elastic constants calculations (Figure S14 and Table S10 in the Supporting Information). Thus, the results reported in this Letter have received an unexpected additional confirmation.

■ ACKNOWLEDGMENTS

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