

Ammonia (NH₃) Production from the Thermal Decomposition of Hydroxylammonium Nitrate (HAN) as a Green Energetic Source for Clean Space

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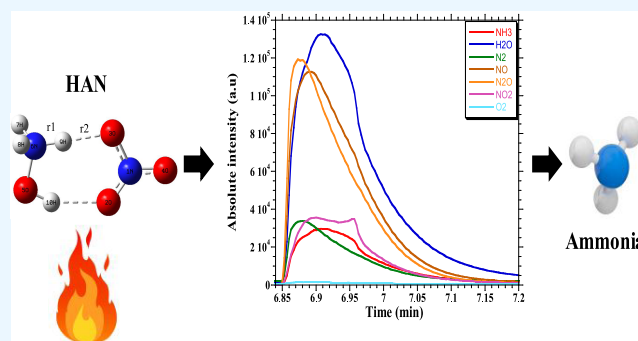
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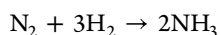
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ABSTRACT: Ammonia's (NH₃) high hydrogen concentration and simplicity of storage and transportation have made it a promising energy source, especially for hydrogen production. Using an iridium (Ir)-based catalyst for clean space applications, this study examines the release of NH₃ during the thermal decomposition of hydroxylammonium nitrate (HAN), a green energetic propellant. Differential thermal analysis-thermogravimetry in conjunction with mass spectrometry (DTA-TG/MS) was used to examine the thermal decomposition. The generation of NH₃ was verified by subsequent fragment analysis. Coupled cluster approaches were utilized to validate NH₃ generation and to further clarify the reaction process. Combining the theoretical and experimental methods highlights the feasibility of employing HAN as a precursor for NH₃ production, indicating that it can be used as a sustainable energy source for space propulsion systems. The effect of temperature on NH₃ production using a coupled cluster is also explored.



INTRODUCTION

Production of NH₃ is an important industrial process that is mostly utilized in the production of fertilizers, which are necessary for contemporary agriculture.^{1–3} The Haber–Bosch process, created in the early 1900s by Fritz Haber and Carl Bosch, is the method most commonly used to synthesize NH₃. In this process, nitrogen (N₂) from the air and hydrogen (H₂), which is commonly obtained from natural gas (methane), are directly combined at high pressures and temperatures with the aid of a catalyst, which is often iron-based.⁴ The following succinctly describes the reaction:



The energy-intensive process of producing NH₃ uses a lot of natural gas to provide the required heat as well as a supply of hydrogen.^{5,6} NH₃ can be obtained from the thermal decomposition of green propellants such as ammonium dinitramide (ADN)^{7,8} and ammonium nitrate (AN).⁹ HAN liquid propellant has been extensively studied recently as a potential replacement for hydrazine, primarily due to its high specific impulse (Isp),^{10–13} which provides superior performance in propulsion applications. Unlike hydrazine, which is known for its high toxicity and handling risks, HAN propellant boasts significantly lower toxicity,^{14,15} making it safer for both humans and the environment. This reduced toxicity also simplifies the handling and storage requirements, reducing the

overall operational costs. Furthermore, HAN has high oxidability,¹⁶ which contributes to its efficiency as a propellant by ensuring complete combustion and reducing the formation of undesirable byproducts. The reactivity of HAN propellant has also been a subject of intense study to understand the behavior of this hazardous material under different conditions.^{17–19} Understanding its reactivity is crucial for safe handling, storage, and usage, as well as for optimizing its performance in propulsion systems. Recent research has delved into the decomposition pathways of HAN, shedding light on the formation of byproducts such as NH₃ and nitric oxide (NO).^{20,21} These studies are essential for developing mitigation strategies for any potential environmental and health impacts resulting from the use of the HAN propellant. The decomposition characteristics not only inform safety protocols but also provide insights into the efficiency and reliability of HAN as a propellant in various aerospace applications. In this paper, NH₃ production from the thermal decomposition of HAN energetic propellant was demonstrated

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by analyzing ejected gases in real time by using a mass spectrometer linked to a differential thermal analysis-thermogravimetry (DTA-TG) technique. Moreover, the coupled cluster (CC) simulation method was employed to demonstrate NH_3 release in the presence of two and three atoms of Ir as a catalyst. NH_3 is an energetic source of green hydrogen (H_2) production free of carbon dioxide (CO_2). Moreover, the production of NH_3 from energetic compounds such as ADN, AN, or HAN propellants is not cost-effective and can be released in the presence of adequate catalysts. The effect of the temperature on NH_3 energy synthesis was also examined and discussed. For this reason, three different temperatures were selected: ambient temperature (298 K), onset temperature of HAN decomposition (338 K), and the temperature at which water as a solvent is removed (373 K). Therefore, the thermal decomposition of binary HAN(73%)-water as a propellant can release NH_3 , which can be generated using an Ir-based catalyst. This catalyst first decomposes the HAN propellant into NH_2OH (an alkaline compound) and HNO_3 (an acidic compound). The Ir catalyst efficiently decomposes the alkaline medium into NH_3 , which can be used as an additive to lower burning rates and specific impulses for reaction control systems (thrusters). The remaining products can be analyzed to assess their effects on catalyst deactivation for long-term use.

EXPERIMENTAL METHOD

The thermal decomposition of HAN ($\text{NH}_2\text{OH}\cdot\text{NO}_3$) propellant in the presence of an Ir-based catalyst was investigated using DTA-TG/MS (Shimadzu, Japan) connected to a mass spectrometer (MS) at 1 atm. The Ir-based catalyst, with the active phase deposited onto SiO_2 -doped Al_2O_3 , was prepared by using wet impregnation. Characterization of this catalyst (not presented here) revealed that nanoparticles with an average diameter of approximately 5 nm were homogeneously distributed throughout the support.

Starting at ambient temperature and increasing to 400 °C, the experiment used a temperature ramp rate of 5 °C/min. With this configuration, it was possible to evaluate mass loss (TG) and thermal effects (DTA) concurrently while the HAN propellant thermally decomposed. MS was used to study the changing gases in real time, giving extensive insights into the paths and products of decomposition. By combining these methods, HAN decomposition's thermal behavior and catalytic effects may be fully understood.

Direct insertion probe mass spectrometry (DIP-MS) L-250G-I A, developed by Canon Anelva Co., Ltd. (Kawasaki, Japan), is utilized for the detailed examination and thermal analysis of HAN-based samples, focusing on their mass composition of HAN and water. This analytical technique involves introducing the sample into the ionization chamber, where it undergoes vaporization and is subsequently ionized through electronic excitation. The DIP-MS system is recognized as the most efficient tool for the real-time identification of gas products during thermal decomposition. Remarkably, it can achieve a temperature increase from 40 to 450 °C, utilizing a rapid temperature ramp of approximately 128 °C/min. This innovative approach has never been previously applied to HAN-based propellants. The probe's temperature program was designed to increase from room temperature to 450 °C at a swift rate of 128 °C/min. During the analysis, we used an ionization voltage of 70 eV, maintained the source temperature at 250 °C, and analyzed

a mass range from $m/z = 17$ to 100. Scans were conducted at a rate of 2 scans per second, with a high-quality vacuum maintained at better than 7×10^{-5} mbar.

THEORETICAL BASIS

The production of NH_3 during the thermal decomposition of the HAN propellant catalyzed by Ir was investigated using the coupled cluster (CC) method. This sophisticated computational method is well-known for accurately characterizing electron correlation, which makes it ideal for researching reaction energetics and processes. Clusters including 2 and 3 Ir atoms were chosen in order to investigate the catalytic effect of Ir on NH_3 synthesis. The HAN molecule was modeled interacting with these clusters in order to assess the energy feasibility and possible paths for NH_3 production. Moreover, in the case of HAN propellant, which is an ionic solution (NH_2OH^+ as cation and NO_3^- as anion), Ir atoms with free d orbitals can easily be linked via dative bonding. The electrical structure, reaction intermediates, transition states, and general energy profiles for the decomposition process were all thoroughly described by the CC calculations. The study sought to determine the best catalytic designs and comprehend the effects of altering the number of Ir atoms on NH_3 generation by analyzing various Ir cluster sizes. This method provided insightful information on how Ir functions to maximize catalytic efficiency and promote the intended reaction. Moreover, three different temperatures were considered to investigate their effects on the production of NH_3 using coupled clusters.

RESULTS AND DISCUSSION

The experimental investigation into the production of NH_3 from the thermal decomposition of HAN propellant was

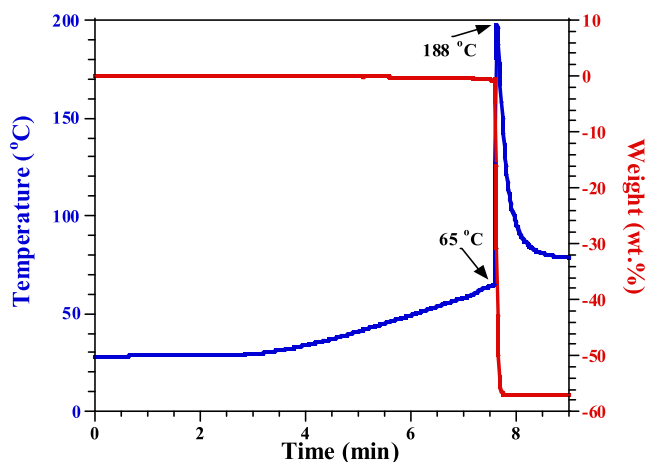


Figure 1. DTA-TG thermogram of the thermal decomposition of the HAN propellant.

conducted using an Ir-based catalyst. In fact, The Ir-based catalyst is unique for the decomposition of HAN to hydroxylamine (NH_2OH) in an alkaline medium and nitric acid (HNO_3) in an acidic medium because it can decompose at a low onset temperature in the presence of Ir particles. Moreover, in the second step, Ir effectively decomposes the alkaline medium to ammonia, which is central to the findings presented in this paper. This study aimed to understand the NH_3 release mechanism and optimize the conditions for its

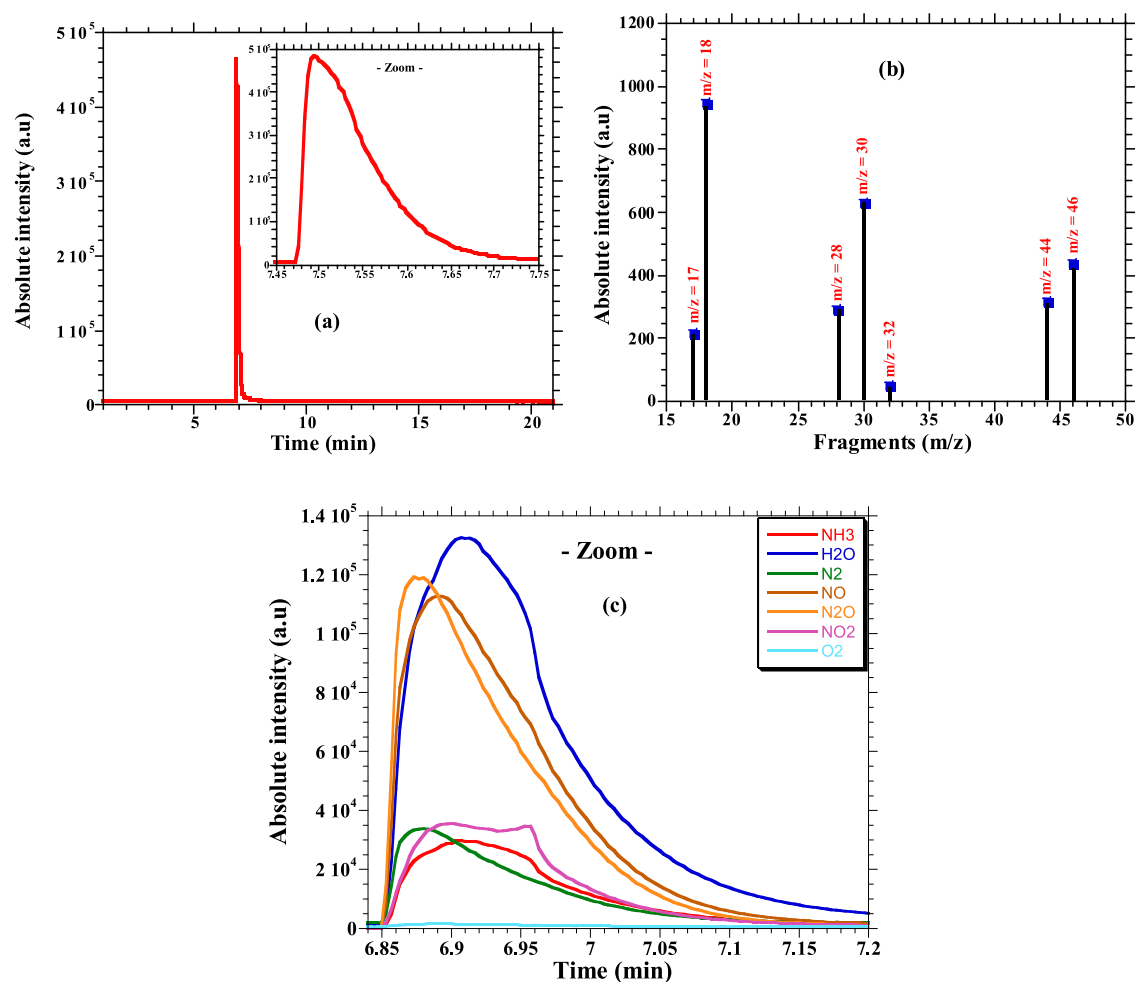


Figure 2. (a) Absolute intensity vs time of the thermal decomposition obtained by MS, (b) obtained fragments (m/z), and (c) real-time analysis of ejected gas by MS.

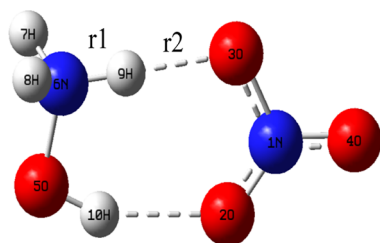


Figure 3. Optimized structure of the HAN propellant.

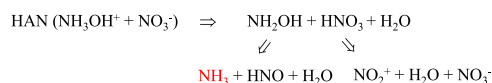


Figure 4. NH_3 production from the decomposition of the HAN propellant.

synthesis. The thermal decomposition process was meticulously analyzed, with a particular focus on the role of the Ir catalyst in facilitating the HAN decomposition using 2 and 3 atoms of Ir. To gain a comprehensive understanding of the NH_3 production mechanism, the coupled cluster method was employed. This advanced computational technique was utilized to perform a detailed mechanism analysis, including the construction of energy diagrams. The study examined how varying temperatures affected the NH_3 synthesis, allowing for a

nuanced exploration of the reaction kinetics and catalytic efficiency. By integrating experimental data with computational simulations, the research provided valuable insights into optimizing the conditions for NH_3 production from the HAN propellant.

Therefore, the thermal decomposition of HAN propellant over Ir-based catalyst was experimentally performed using DTA-TG/MS techniques as shown in [Figure 1](#).

From this figure, Ir is capable of exothermally decomposing HAN in a single step at a low temperature of around 65 °C as an onset temperature with a maximum of 188 °C reached out in the Al-cell, which is in contrast to the decomposition observed with HAN-free catalysts.²² A strong, intense peak was observed during this process.

The thermal decomposition of the HAN energetic propellant was performed after that using a real-time analysis by MS, and the obtained data are illustrated in [Figure 2](#).

A real-time analysis of the ejected gas from the HAN propellant, conducted in the presence of Ir particles as a catalyst, enabled us to distinctly identify the various species associated with the mass fragments (m/z). The use of Ir particles facilitated a catalytic reaction environment, leading to a more nuanced separation and identification of different gas species. By monitoring the mass-to-charge ratios of the ejected fragments, we were able to precisely distinguish between the different natures of the chemical species present. This

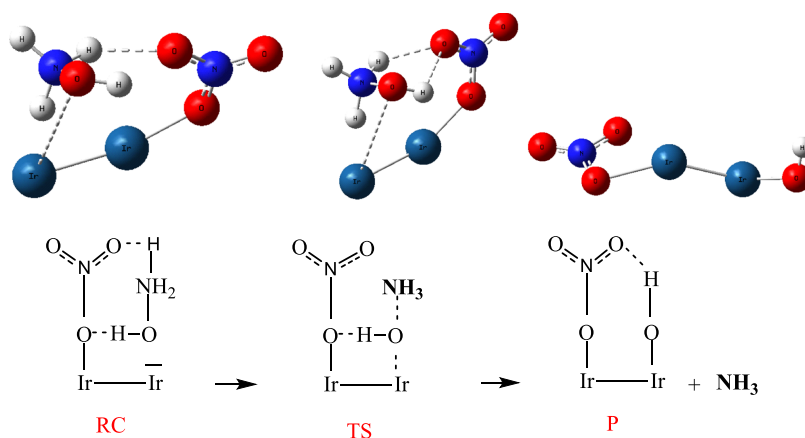


Figure 5. Coupled cluster for NH_3 production from HAN decomposition using 2 atoms of Ir.

Table 1. Relative Energies and Energy Barriers (kcal mol^{-1}) of NH_3 Production from HAN Decomposition in the Presence of Two Ir Atoms

reaction	$T = 298 \text{ K}$		$T = 338 \text{ K}$		$T = 373 \text{ K}$	
	ΔG	E_a	ΔG	E_a	ΔG	E_a
$\text{RC} \rightarrow \text{P1} + \text{NH}_3$	-64.02	0.54	-65.26	0.74	-66.35	0.92

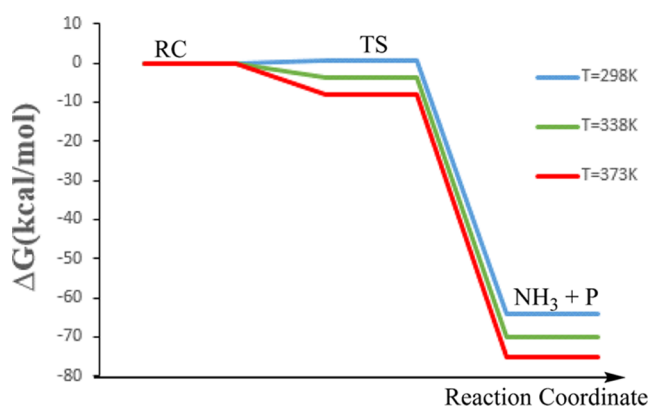


Figure 6. Energetic diagram of NH_3 production from HAN-2Ir decomposition at different temperatures: $T = 298, 338$, and 373 K .

approach provided valuable insights into the reaction dynamics and the specific roles of the catalyst in modifying the propellant's decomposition profile.

The gases ejected after the thermal decomposition of HAN were analyzed by MS. The release of NH_3 was confirmed by the appearance of the $m/z = 17$ fragment (Figure 2b). The MS analysis is presented in Figure 2a. As observed, the thermal decomposition of HAN propellant with Ir as a catalyst is a violent exothermic process, occurring in one step as previously reported.^{22,23} The completed analyzed gases were presented in Figure 2c, and the different fragments were attributed to nitrogen (N_2), NO_x , vapor steam, and NH_3 .

On the other hand, in this study, experimental data on the NH_3 production from the decomposition of HAN propellant using iridium particles as a catalyst, along with the analysis of different ejected gases via MS, are presented. These experimental observations provide valuable insights into the catalytic processes and the nature of the reactions involved. To theoretically elucidate these findings, we next examine the reaction mechanisms involving HAN and Ir atoms using the coupled cluster method. This advanced computational

technique allows for an in-depth analysis of the electronic structure and reaction pathways, offering a detailed understanding of how Ir particles facilitate the decomposition of HAN and influence NH_3 production. By correlating the theoretical predictions with the experimental data, we aim to provide a comprehensive explanation of the catalytic processes observed, thus bridging the gap between empirical results and theoretical models. Figure 3 illustrates the optimized structure of HAN propellant in its ionic liquid state, i.e., hydroxylammonium (NH_3OH^+) as cation and nitrate (NO_3^-) as anion.

Moreover, the thermal decomposition of HAN propellant has been previously discussed, and most research groups believe that the main products of the first step were hydroxylamine (NH_2OH) and nitric acid (HNO_3) dissolved in water^{18,24,25} as shown in Figure 4.

NH_2OH then rearranges to produce NH_3 , HNO , and water, while HNO_3 decomposes into NO_2^+ , NO_3^- , and water. Therefore, the HAN propellant is considered a good source to produce NH_3 for different applications.

The coupled cluster method was used to correlate NH_3 release from HAN decomposition in the presence of two Ir atoms as shown in Figure 5.

In this case, the optimized HAN-2Ir (top left), so-called reaction coordinate (RC), was oriented in the direction to realize the interaction between two oxygen atoms from NH_3OH^+ to NO_3^- , respectively, with both Ir atoms. This mechanism begins with the NH_3 production from the RC complex (HAN adsorbed on Ir atoms) via the transition state (TS). The resulting product, so-called P, then undergoes a rearrangement by the migration of hydrogen from the hydroxyl (OH) group bound to the Ir atom and the oxygen (O) of the nitrous oxide (NO_2) group. At the same time, the evaluation of the temperature's effect on NH_3 production from HAN decomposition was carried out. The results of this study are given in Table 1 and depicted in Figure 6.

From Table 1 and Figure 6, it is evident that NH_3 synthesis via the thermal decomposition of HAN propellant is

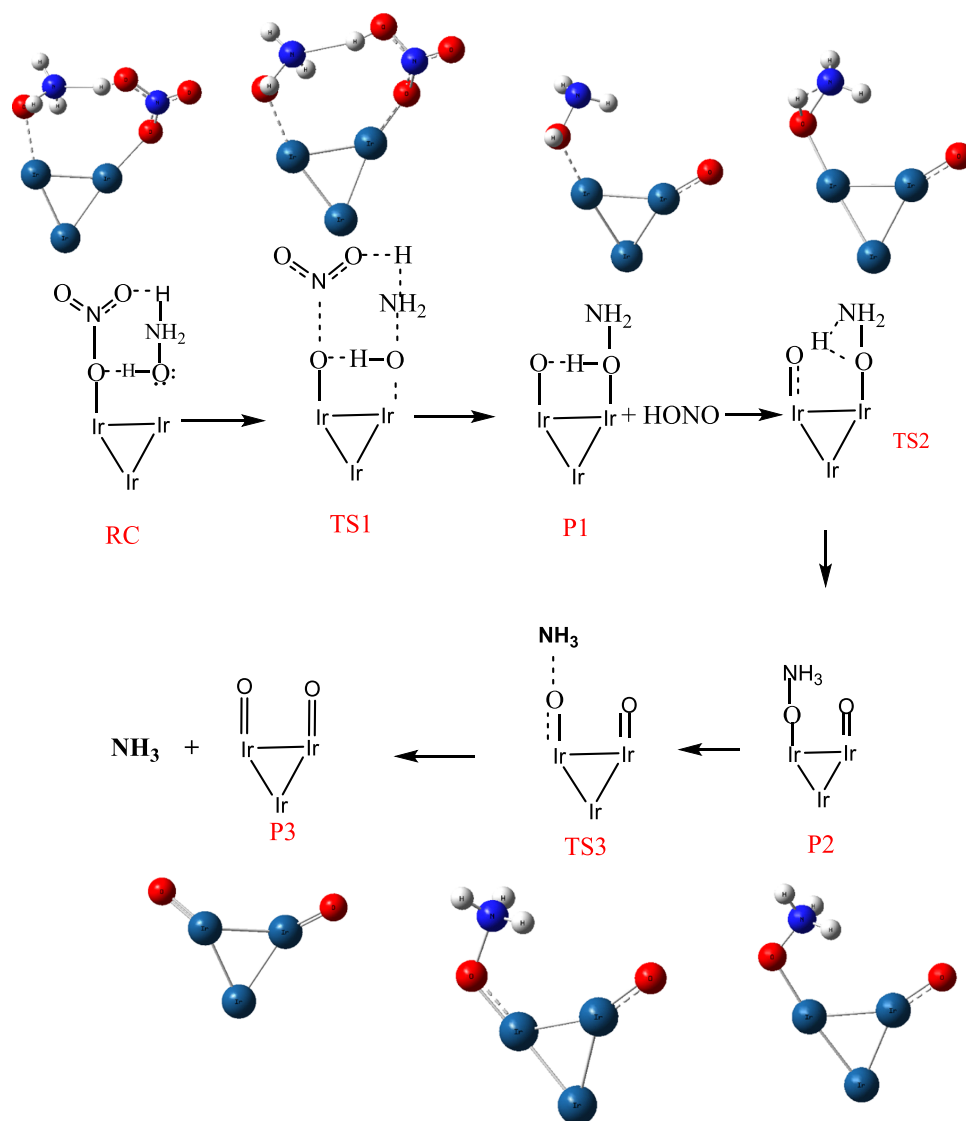


Figure 7. Coupled cluster for NH_3 production from HAN decomposition using 3 atoms of Ir.

Table 2. Relative Energies and Energy Barriers (kcal mol^{-1}) of NH_3 Production from HAN Decomposition in the Presence of Three Ir Atoms

reactions	$T = 298 \text{ K}$		$T = 338 \text{ K}$		$T = 373 \text{ K}$	
	ΔG	E_a	ΔG	E_a	ΔG	E_a
$\text{RC} \rightarrow \text{P1} + \text{HONO}$	-32.06	6.58	-33.90	6.60	-35.51	6.63
$\text{P1} \rightarrow \text{P2}$	-2.85	29.50	-2.82	29.56	-2.79	29.62
$\text{P2} \rightarrow \text{P3} + \text{NH}_3$	-30.44	7.684	-31.72	7.73	-32.84	7.78

accompanied by a free energy change ($\Delta G < 0$), confirming the thermodynamic feasibility of the process. This reaction can be accelerated with increasing temperatures. The RC, as the initial interactive complex, is stable. However, the free energy (ΔG) of the TS intermediate structure decreases, indicating that the NH_3 production becomes thermodynamically more favorable at higher temperatures.

The effect of the number of Ir atoms for NH_3 synthesis from the thermal decomposition of the HAN propellant was performed. At this time, three atoms were chosen to react with the HAN structure, and the obtained data are illustrated in Figure 7.

Three iridium (Ir) atoms (HAN-3Ir) engage with the oxygen (O) atom of the NH_3OH^+ cation and oxygen (O) atom of the NO_3^- anion in this reaction. The rearrangement of the intermediate TS1 complex was followed by the release of nitrous acid (HONO), as shown by the improved reaction mechanism. The resulting P2 intermediate complex then goes through a further rearrangement to reach the TS3 state. The stable gas NH_3 can then be produced by the breakdown of this TS3 complex. Because we could synthesize NH_3 in a single step in the first example, the release of NH_3 was easier from both the 2 Ir and 3 Ir atoms. Nevertheless, 3 Ir atoms were used in the second stage to produce NH_3 . Consequently, a low Ir-concentrated catalyst might be sufficient for NH_3 synthesis.

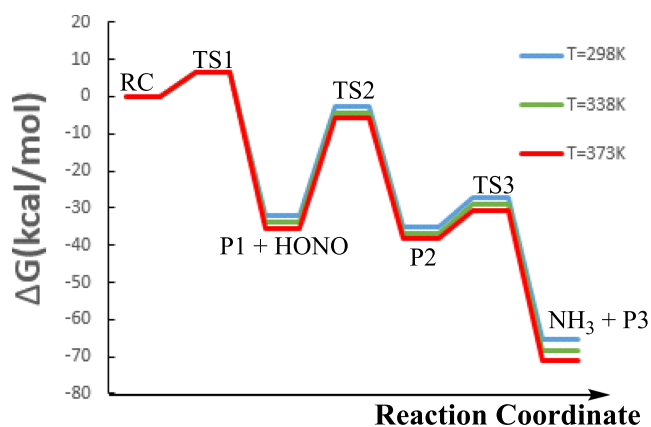


Figure 8. Energetic diagram of NH_3 production from HAN-3Ir decomposition at different temperatures: $T = 298$, 338 , and 373 K.

The effect of temperature on the thermal decomposition of the HAN-3Ir system was evaluated, and the findings are represented in Table 2 and Figure 8.

According to the data that are shown, the HAN-3Ir system's thermal decomposition becomes somewhat more preferred as the temperature rises. Actually, there was a 2 kcal mol^{-1} acceleration of the first reaction, $\text{RC} \rightarrow \text{P1} + \text{HONO}$. The second stage involved the synthesis of NH_3 , and once more, the temperature rising had a favorable impact on the synthesis of NH_3 from the thermal decomposition of HAN-3Ir. It can be concluded that a theoretical study utilizing the coupled cluster method has demonstrated that NH_3 can be produced from the thermal decomposition of HAN propellant when catalyzed by a low Ir-concentrated catalyst. The research examined the influence of Ir atom numbers and the initial temperatures of the reactions. These simulations aimed to corroborate experimental findings obtained through the DTA-TG/MS technique. The experimental results, which identified ejected gas species from HAN decomposition in real time, were successfully supported by the theoretical data, confirming that a low Ir-concentrated catalyst facilitates NH_3 production under the specified conditions.

CONCLUSIONS

The potential for producing NH_3 through the thermal breakdown of HAN as a source for space applications is examined in this study. The formation of NH_3 was demonstrated by the experimental data obtained by using the DTA-TG/MS approach when Ir particles were used as a catalyst. Computational investigations that investigated the interaction of HAN with two and three Ir atoms, using the coupled cluster approach, further validated these experimental data. The computational results showed that two oxygen atoms must be close to the Ir atoms in order for NH_3 to be produced. The investigation also discovered that increasing the temperature thermodynamically supported the processes that produced NH_3 at low free energies. The significance of catalyst design and heat conditions in enhancing the generation of NH_3 from HAN is underscored by these findings, which provide encouraging perspectives for the creation of sustainable energy sources for clean space propulsion systems.

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Author Contributions

The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript.

Notes

The authors declare no competing financial interest.

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ABBREVIATIONS

HAN, hydroxylammonium nitrate; RC, reaction coordinate; TS, transition state; DTA, differential thermal analysis; TG, thermogravimetric; MS, mass spectrometer; Ea, activation energy; CC, coupled cluster

REFERENCES

- (1) Ishaq, H.; Crawford, C. Review and evaluation of sustainable ammonia production, storage and utilization. *Energy Convers. Manage.* **2024**, *300*, No. 117869.
- (2) Ghavam, S.; Vahdati, M.; Wilson, I. A. G.; Styring, P. Sustainable Ammonia Production Processes. *Front. Energy Res.* **2021**, *9*, No. 580808.
- (3) Valera-Medina, A.; Valera-Medina, A.; Amer-Hatem, F.; Azad, A.; Dedoussi, I.; De Joannon, M.; Fernandes, R.; Glarborg, P.; Hashemi, H.; He, X.; Mashruk, S.; McGowan, J.; Mounaim-Rouselle, C.; Ortiz-Prado, A.; Ortiz-Valera, A.; Rossetti, I.; Shu, B.; Yehia, M.; Xiao, H.; Costa, M. Review on Ammonia as a Potential Fuel: From Synthesis to Economics. *Energy Fuels* **2021**, *35* (9), 6964–7029.
- (4) Smith, C.; Hill, A. K.; Torrente-Murciano, L. Current and future role of Haber–Bosch ammonia in a carbon-free energy landscape. *Energy Environ. Sci.* **2020**, *13* (2), 331–344.
- (5) Andriani, D.; Bicer, Y. A Review of Hydrogen Production from Onboard Ammonia Decomposition: Maritime Applications of Concentrated Solar Energy and Boil-Off Gas Recovery. *Fuel* **2023**, *352*, No. 128900.
- (6) Juangsa, F. B.; Irhamna, A. R.; Aziz, M. Production of ammonia as potential hydrogen carrier: Review on thermochemical and electrochemical processes. *Int. J. Hydrogen Energy* **2021**, *46* (27), 14455–14477.
- (7) Harimech, Z.; Toshtay, K.; Atamanov, M.; Azat, S.; Amrousse, R. Thermal Decomposition of Ammonium Dinitramide (ADN) as

Green Energy Source for Space Propulsion. *Aerospace* **2023**, *10* (10), No. 832.

(8) Kumar, P. An overview on properties, thermal decomposition, and combustion behavior of ADN and ADN based solid propellants. *Defence Technol.* **2018**, *14* (6), 661–673.

(9) Cagnina, S.; Rotureau, P.; Fayet, G.; Adamo, C. The ammonium nitrate and its mechanism of decomposition in the gas phase: a theoretical study and a DFT benchmark. *Phys. Chem. Chem. Phys.* **2013**, *15* (26), 10849–10858.

(10) Amrousse, R.; Hori, K.; Fetimi, W.; Farhat, K. HAN and ADN as liquid ionic monopropellants: Thermal and catalytic decomposition processes. *Appl. Catal., B* **2012**, *127*, 121–128.

(11) Bao, L.; Wang, H.; Wang, Z.; Xie, H.; Xiang, S.; Zhang, X.; Zhang, W.; Huang, Y.; Shen, R.; Ye, Y. Controllable ignition, combustion and extinguishment characteristics of HAN-based solid propellant stimulated by electric energy. *Combust. Flame* **2022**, *236*, No. 111804.

(12) Ferguson, R. E.; Shafirovich, E. Combustion of Gelled HAN/Methanol/Water Propellants. *Propellants, Explos., Pyrotech.* **2021**, *46* (11), 1672–1678.

(13) Agnihotri, R.; Oommen, C. Cerium oxide based active catalyst for hydroxylammonium nitrate (HAN) fueled monopropellant thrusters. *RSC Adv.* **2018**, *8* (40), 22293–22302.

(14) Hori, K.; Katsumi, T.; Sawai, S.; Azuma, N.; Hatai, K.; Nakatsuka, J. HAN-Based Green Propellant, SHP163 – Its R&D and Test in Space. *Propellants, Explos., Pyrotech.* **2019**, *44* (9), 1080–1083.

(15) Chai, W. S.; Cheah, K. H.; Wu, M.-H.; Koh, K. S.; Sun, D.; Meng, H. A review on hydroxylammonium nitrate (HAN) decomposition techniques for propulsion application. *Acta Astronaut.* **2022**, *196*, 194–214.

(16) Markandan, K.; Zhang, Z.; Chin, J.; Cheah, K. H.; Tang, H.-B. Fabrication and preliminary testing of hydroxylammonium nitrate (HAN)-based ceramic microthruster for potential application of nanosatellites in constellation formation flying. *Microsyst. Technol.* **2019**, *25* (11), 4209–4217.

(17) Zhu, Q.; Lei, X.; Liu, B.; Hu, Z.; Xu, Q.; Pan, Y.; Hou, B.; Wang, X.; Wang, Z. Experimental and Theoretical Studies of HAN and HEHN Pyrolysis at Low Pressure. *Energy Fuels* **2024**, *38* (7), 6370–6378.

(18) Izato, Y.-I.; Koshi, M.; Miyake, A. Decomposition Pathways for Aqueous Hydroxylammonium Nitrate Solutions: a DFT Study. *Cent. Eur. J. Energ. Mater.* **2017**, *14* (4), 888–916.

(19) Zhou, X.; Wang, Q.; Shi, Z.; Hu, X.; Yao, T.; Huang, Y. A theoretical investigation of the catalytic decomposition of hydroxylamine nitrate on Ir(1 1 0) surface. *Comput. Theor. Chem.* **2023**, *1225*, No. 114141.

(20) Chambreau, S. D.; Popolan-Vaida, D. M.; Vaghjiani, G. L.; Leone, S. R. Catalytic Decomposition of Hydroxylammonium Nitrate Ionic Liquid: Enhancement of NO Formation. *J. Phys. Chem. Lett.* **2017**, *8* (10), 2126–2130.

(21) Taylor, N. R.; Brummel, M. H.; Mooney, M. M.; Kerber, T. V.; Lemmer, K. M. On the formation of ammonia from the thermal decomposition of hydroxylammonium nitrate vapor. *J. Ionic Liq.* **2024**, *4* (1), No. 100083.

(22) Amrousse, R.; Katsumi, T.; Azuma, N.; Hori, K. Hydroxylammonium nitrate (HAN)-based green propellant as alternative energy resource for potential hydrazine substitution: From lab scale to pilot plant scale-up. *Combust. Flame* **2017**, *176*, 334–348.

(23) Amrousse, R.; Katsumi, T.; Itouyama, N.; Azuma, N.; Kagawa, H.; Hatai, K.; Ikeda, H.; Hori, K. New HAN-based mixtures for reaction control system and low toxic spacecraft propulsion subsystem: Thermal decomposition and possible thruster applications. *Combust. Flame* **2015**, *162* (6), 2686–2692.

(24) Zhang, K.; Thynell, S. T. Thermal Decomposition Mechanism of Aqueous Hydroxylammonium Nitrate (HAN): Molecular Simulation and Kinetic Modeling. *J. Phys. Chem. A* **2018**, *122* (41), 8086–8100.

(25) Banerjee, S.; Shetty, S. A.; Gowrav, M. N.; Oommen, C.; Bhattacharya, A. Adsorption and decomposition of monopropellant

molecule HAN on Pd(100) and Ir(100) surfaces: A DFT study. *Surf. Sci.* **2016**, *653*, 1–10.



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