# Oxidative Dehydrogenation of Propane on the Oxygen Adsorbed Edges of Boron Nitride Nanoribbons

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# Point-by-point reply to the reviewers' comments

**REVIEWER REPORT(S):**

**Referee: 1**

Comments:

The authors have addressed the main comments of both Reviewers and I can recommend publication after this minor comment is addressed. In particular, regarding point 2 of Reviewer 1, the authors poorly included in the revised manuscript the discussion on which and how other products (especially coking) are formed. I believe that a discussion, together with error-dependent selectivity change (a 95%-to-80% drop is considerable for an error of just 0.1 eV!) should be expanded in the re-amended manuscript, as they did in the reply, for clarity and transparency.

**Authors' reply:** As suggested by the reviewer, we have added the following discussion on the page 25 of the revised manuscript: *"Thus, at similar propane ($C_3H_8$) and propene ($C_3H_6$) partial pressures, the selectivity to propene (versus propene activation products such as $C_2H_4$ and $CO_x$) can be estimated from $\frac{r_{propene}^{consumption}}{r_{propene}^{production}} = e^{\left(\frac{-(\Delta G_{C3H6}^{TS} - \Delta G_{C3H8}^{TS})}{k_B T}\right)}$, where $\Delta G_{C3H6}^{TS} - \Delta G_{C3H8}^{TS}$ is the difference between the free energy barriers of propene and propane activation, respectively. For a free energy barrier difference of 0.2 eV, we obtain a propene selectivity of ~95% at 800 K. This indicates that the considered $N_2O/NO_x$ active site on the BN edge is indeed selective for the propene production. As a word of caution, we note that if the difference in activation barrier is only 0.1 eV (which is certainly within the uncertainty range of DFT), then the predicted propene selectivity at equal partial pressures of propane and propene would only be ~80%. In other words, it is very challenging to accurately quantify all reaction products from the $N_2O/NO_x$ type active site. Also, the proposed catalyst is expected to generate $C_3H_7$• radicals that can trigger gas phase reactions as experimentally speculated and that can dissociate to into the experimentally observed $C_2H_4$ and $CH_3$• radical."*

# Oxidative Dehydrogenation of Propane on the Oxygen Adsorbed Edges of Boron Nitride Nanoribbons

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1

## ABSTRACT:

Metal-free boron nitride has recently been reported to exhibit high catalytic activity and selectivity towards oxidative dehydrogenation of propane (ODHP). Despite several experimental studies, the exact nature and function of the active sites in this emerging catalyst are unknown. In the present work, density functional theory calculations are combined with microkinetic modeling to systematically explore the ODHP on oxygen passivated boron nitride nanoribbons (BNNRs). The relative stabilities of different edge structures of BNNR were examined using *ab initio* thermodynamic analysis, and the most stable oxygen passivated edge structure was used for a mechanistic study. Microkinetic analysis revealed that a $N_2O$ or $NO_x$-type active site is active and selective for the conversion of propane to propene. In addition to a heterogeneous catalytic cycle, the proposed $N_2O/NO_x$-type active sites are expected to be able to generate gas phase $C_3H_7^{\bullet}$, which in turn can trigger gas phase reactions of ODHP as experimentally speculated.

## 1. INTRODUCTION

Recently, the oxidative dehydrogenation of propane (ODHP) has attracted immense research interest for producing one of the most important light olefins in the petrochemical industry, propene. The ODHP promises a significant improvement in terms of energy consumption,[1, 2] catalyst stability (lack of coke formation),[3] and propane conversion,[4] over on-purpose non-oxidative catalytic processes and conventional non-oxidative cracking processes of naphtha.[5, 6]

However, the selectivity towards propene in ODHP catalyzed by transition metal oxides and alkaline-earth metal is poor. This is largely due to the over-combustion of the reaction product propene to $CO_x$.[7-12] The ODHP over a $VO_x/CaO-\gamma-Al_2O_3$ (1:1) catalyst under gas phase, oxygen-

free conditions, i.e., using lattice oxygen, shows promising activity with high propane conversion (65%) and propene selectivity (85%). However, it also produces considerable amounts of $CO_2$ (selectivity ~15%) and requires the setup of at least two reactors (a reactor and a catalyst regenerator).[13]

In this context, hexagonal boron nitride (h-BN) has recently appeared as a potential metal-free catalyst for ODHP with comparable propene selectivity to that of the above-mentioned vanadium oxide catalyst, but with only negligible $CO_2$ formation even in the presence of molecular oxygen. Grant et al. reported that h-BN offers 79% selectivity towards propene at 14% propane conversion with negligible $CO_2$ formation when heated to 460-500 °C under flowing propane, oxygen, and nitrogen gas.[14] As the observed activity is still low, a deeper understanding of the active site and reaction mechanism of the ODHP over h-BN is needed to optimize this catalyst system. Many mechanisms and active sites have been proposed for this reaction. By comparing *ab initio* modeled wavenumbers to experimental spectroscopic findings, Grant et al. proposed that the molecular oxygen adsorbed armchair edge of h-BN acts as the active site for the ODHP reaction.[14] In addition, they suggested that the ODHP reaction can be initiated with secondary hydrogen abstraction from propane by a B–O–O–N active site, leading to a surface-stabilized propyl intermediate with adjacent B–OH species.[14] Next, Shi et al. reported that the zigzag edge of h-BN with attached B–OH groups can efficiently catalyze the ODHP reaction with superior propene selectivity (80.2%) at a remarkable propane conversion (20.6%) and with negligible production of $CO_2$ (selectivity 0.5%).[15] They proposed a radical type mechanism where the active site is a BNO$^\bullet$ species, generated by molecular oxygen abstracting a hydrogen from B–OH groups, which can trigger propane dehydrogenation.[15-18] In other recent work, Hermans et al. hypothesized that the high selectivity towards propene under ODHP reaction conditions is not unique for only BN, but is similar for many boron-containing materials such as: boron carbide, titanium boride, nickel

boride, cobalt boride, hafnium boride, tungsten boride, and elemental boron.[19, 20] As they found elemental boron as the most efficient catalyst among the tested boron containing materials, they concluded that boron is the essential element for achieving high propene selectivity. Indeed, they proposed a surface-stabilized $BO_x$ or $B(OH)_xO_{3-x}$ species as the active site for the ODHP, which contradicts their previous h-BN edge site mechanistic hypothesis.[19-21] Using SiC as an inert catalyst diluent, Venegas and Hermans furthermore hypothesized that gas-phase chemistry has a significant influence on the ODHP reaction over h-BN.[22] They speculated that their previously proposed[19, 20] $BO_x$ active sites on h-BN act as "initiators" that can generate propyl radicals by snatching an H atom from propane, which again, can trigger radical chain reactions through interaction with oxygen, leading to a gas phase mechanism for the ODHP reaction.[22] Interestingly and somewhat contradictory to the interpretation of experimental data from Hermans et al., Chaturbedy et al. found that the oxidation of B-N bonds in h-BN poisoned the catalyst.[23] They observed an initially high catalytic activity of h-BN, which provided remarkable selectivity for alkenes (~70%) at very high conversion (~50%) of propane, but h-BN retained this activity for only 5 hours. According to Chaturbedy et al., the short catalyst lifetime appeared to be due to oxidation of surface B−N bonds, which can be reduced by heating in ammonia. Next, Chaturbedy et al. hypothesized various B−N species on the BN surface and/or edge, such as B−N, B−N−B, N−B−N, and B−NH₂, as the active sites for the ODHP reaction.[23] The potential importance of N- or $NO_x$-type active sites bound to boron atoms is further motivated by experimental results from Annamalai et al. who observed that gas-phase $NO_x$-species can catalyze the ODHP with very high selectivity.[24]

In other words, there is no consensus in the community over what is the active site and reaction mechanism. In addition, all the above-mentioned experiments were carried out under high

concentrations of nitrogen gas ($N_2$) and elevated temperatures (~500 °C) during which BN can react and form various surface sites. For example, Grant et al.[19] performed the ODHP reaction on a number of boron containing materials including elemental boron at 500 °C with a gas concentration ratio of 3:6:11 of $O_2$:$C_3H_8$:$N_2$. We hypothesize that molecular $N_2$ can, at significant concentration and temperature conditions, play a role in creating some kind of nitrogen rich and/or $NO_x$-type active site for ODHP, even when the original material is free of nitrogen, as found in other high temperature reactions.[25, 26] This is in particular possible if the N≡N does not have to be broken for the creation of these sites as will be the case for the active site models studied here.

Thus, given that our understanding of the active site and mechanism for the ODHP reaction on h-BN remains incomplete despite a number of experimental and computational studies,[14-21, 23, 27-29] we have systematically explored the ODHP reaction on oxygen passivated boron nitride nanoribbons (BNNRs) using a combination of DFT and microkinetic modeling techniques. Specifically, we selected a one-dimensional (1D) BNNR active site model, i.e., not a two-dimensional (2D) h-BN cluster model, since the effects of system size are more easily controlled when applying the periodic boundary condition in one direction. We note that it is still possible to study various edge sites that might form under experimental ODHP reaction conditions with BNNR models. Next, we performed an *ab initio* thermodynamic analysis of the different BNNR edge sites in the presence of molecular $O_2$ in order to identify the most stable active sites under experimental ODHP conditions which can be different to the sites available during synthesis conditions and which likely involve some form of oxygen passivation. Then, we studied various reaction pathways on the most stable oxygen passivated active sites and computed free energy diagrams for the surface-catalyzed ODHP. Finally, we developed a microkinetic reaction model for the active site models to predict the turnover frequency, apparent activation barrier, reaction

orders, dominant reaction pathways, and rate controlling elementary steps under ODHP reaction conditions.

## 2. MODELS AND METHODS

### 2.1. Details of Computation.

All periodic DFT calculations of this study were performed using the Vienna *ab initio* simulation package (VASP 5.4).[30, 31] The Perdew, Burke and Ezhernof (PBE)[32] functional was used to describe the exchange and correlation terms of DFT, while core electronic states were described by projected augmented wave (PAW)[33] potentials. The energy cutoff for the plane wave basis sets was 400 eV. To sample the Brillouin zone of a 2D h-BN monolayer, a 3×3×1 Monkhorst-Pack (MP)[34] k-mesh was used, while the k-mesh used for zigzag and armchair BNNRs were 3×1×1 and 1×3×1, respectively. For geometry optimization, the atomic positions were relaxed until the residual force on each atom became less than 0.01 eV/Å, and the self-consistent field (SCF) energy convergence cutoff was set as $10^{-7}$ eV with a Gaussian smearing of 0.05 eV. A vacuum distance of 15 Å was added normal to the plane to avoid any interaction between the replicas. Since dispersion interactions can play a vital role in the accurate prediction of the energetics of adsorption and desorption processes of long-chain hydrocarbon molecules and considering that the PBE functional is unable to describe van der Waals interactions, we also performed calculations using Grimme's semi-empirical DFT-D3 methodology.[35] Furthermore, we examined the effect of selection of DFT functional on the ODHP reaction by performing select calculations with the newly developed meta-GGA SCAN+rVV10 functional.[36, 37] Overall, we found PBE results to be closer to SCAN+rVV10 results such that in the following we focus on the PBE data. Section 3.3 discusses the effect of DFT functional and D3 correction in more detail.

To model the desired nanoribbons, a large (16×16) orthorhombic 2D supercell of h-BN (a = 40.08 Å and, b = 34.72 Å) as shown in Figure 1(a) was built, starting with the hexagonal unit cell of h-BN with a lattice constant of 2.50 Å. The 1D BNNRs were modeled from this supercell by cutting it in such a way that it produces: (1) an armchair edge (armBNNR), (2) a zigzag edge (zzBNNR), and (3) a modified zigzag edge (mzzBNNR) with boron dangling bonds in one zigzag edge and nitrogen dangling bonds in the other zigzag edge, as shown in Figures 1(b), 1(c), and 1(d), respectively. Each supercell of BNNR possesses 128 atoms (64 B and 64 N) and a fixed lattice constant along the 1D periodic direction in accordance (exactly half) with the corresponding 2D supercell periodic direction. After optimization, the N dangling bonds of mzzBNNR form five-membered rings at the edge as shown in Figure 1(d). The boron and nitrogen dangling bonds of bare BNNRs were passivated by adding O atoms and the stable structures were identified using an *ab initio* thermodynamic analysis. To determine the transition state (TS) of each elementary reaction step we use the climbing-image nudged elastic band (NEB),[38, 39] and the dimer methods.[40, 41] The characterization of all the TS as well as minima were done by numerical vibrational frequency calculations with a step length of 0.02 Å.

## 2.2. *Ab Initio* Thermodynamic Analysis.

The formation of the edge-oxygenated BNNR under ODHP reaction condition was described as BNNR + $\frac{n}{2}$ O₂ → BNNRnO, and the corresponding Gibbs free energies were calculated by,

$$\Delta G_{ads} = E_{BNNRnO}^{ZPE} - E_{BNNR}^{ZPE} - \frac{n}{2} G_{O_2} \tag{1}$$

where $E_{BNNRnO}^{ZPE}$ and $E_{BNNR}^{ZPE}$ correspond to zero-point energy (ZPE) corrected total energies of oxygen adsorbed BNNR and bare armchair BNNR, respectively. The Gibbs free energies of the gas molecules were calculated using,

$$G_{gas}(T,P) = E_{gas}^{DFT} + \Delta\mu_{gas}(T,P^0) + k_B T ln(\frac{P}{P^0}) \tag{2}$$

where $E_{gas}^{DFT}$ is the DFT calculated energy using the PBE-D3 functional, and $\Delta\mu_{gas}(T,P^0)$ is the gas chemical potential calculated from the rotational, translational and vibrational partition functions of the gas molecules. To avoid the well-known errors associated with using DFT−PBE (self-interaction, spin contamination, etc.), the energy of an oxygen molecule, $E_{O_2}$, is obtained semi-empirically from the H$_2$O splitting reaction using the experimental reaction energy and DFT energies of H$_2$ and H$_2$O in the gas phase as,[42, 43]

$$E_{O_2} = 2\left[\left(E_{H_2O}^{DFT} + E_{H_2O}^{ZPE}\right) - \left(E_{H_2}^{DFT} + E_{H_2}^{ZPE}\right) - E_{hof}\right] - E_{O_2}^{ZPE} \tag{3}$$

Here, $E^{ZPE}$ is the experimental zero-point energy,[44] $E_{hof}$ is the experimental heat of formation of a gas-phase H$_2$O molecule (T = 0 K), and $E^{DFT}$ is the energy calculated with the PBE functional.

## 2.3. Microkinetic Modeling.

We used harmonic transition state theory to calculate rate constants for the elementary surface reactions, while collision theory with a sticking coefficient of 1 was used to calculate the rate constants for adsorption processes.

The forward ($k_{for}$) and reverse ($k_{rev}$) rate constants of a surface reaction were calculated as,

$$k_{for} = A_{for}\ e^{\frac{-E_{for}^a}{k_B T}} \ \ and\ \ k_{rev} = A_{rev}\ e^{\frac{-E_{rev}^a}{k_B T}}$$

8

where $E_{for}^a$ and $E_{rev}^a$ correspond to ZPE corrected forward and reverse activation barriers, respectively. The ZPE was calculated from vibrational frequencies ($\nu_i$) as,

$$ZPE = \sum \frac{1}{2} h\, \nu_i$$

The frequency factors ($A_{for}$ and $A_{rev}$) were calculated from the vibrational partition functions ($q_{vib}$) for a certain surface reaction (say A* → B*) as,

$$A_{for} = \frac{k_B T}{h} \frac{q_{vib,TS}}{q_{vib,A*}} \quad \text{and} \quad A_{rev} = \frac{k_B T}{h} \frac{q_{vib,TS}}{q_{vib,B*}}$$

where,

$$q_{vib} = \prod_i \frac{1}{1 - e^{\frac{-h\nu_i}{k_B T}}}$$

To improve the accuracy of the harmonic approximation we shifted all (real) frequencies below 50 cm$^{-1}$ to 50 cm$^{-1}$, so that for surface reactions low frequency modes have no effect on reaction energies and rate constants.

For an adsorption process, the forward rate constant was calculated using

$$k_{for} = \frac{10^5}{\sqrt{2\pi m_A k_B T}} S_{unit} \quad (\text{s}^{-1}\text{atm}^{-1})$$

where $m_A$ is the molecular weight of adsorbed species A and $S_{unit}$ is the adsorption area of the active site. The reverse rate constant ($k_{rev}$) was obtained from the equilibrium constant, $K = \frac{k_{for}}{k_{rev}}$, which was calculated from the ZPE corrected adsorption energy ($\Delta E_{ads}$) and the entropy factors of a gas molecule A using the expression

$$K = \frac{q_{vib,A*}}{q_{vib,*}(q_{vib}q_{rot}q_{trans})_A} e^{\frac{-\Delta E_{ads}}{k_B T}}$$

where A* represents the adsorbed gas species.

After obtaining the forward and reverse rate constants for each elementary reaction, a Master equation was constructed and solved for the steady-state solution of probability densities for the system to occupy each discrete state, referred to as surface coverage ($\theta$), which in turn provides turnover frequencies (TOF).

The apparent activation energy ($E_{app}$) was calculated as,

$$E_{app} = RT^2 \left( \frac{d \ln r_{overall}}{dT} \right)_{P, y_i}$$

from the overall rates keeping the total pressure ($P$) and the mole fraction of species i in the reaction mixtures ($y_i$) constant.

To determine the reaction order ($\alpha_i$) with respect to species i at a specific temperature (T) we used the expression

$$\alpha_i = \left( \frac{d \ln r_{overall}}{d \ln p_i} \right)_{T, p_{j \neq i}}$$

where the partial pressure of the species ($p_i$) was varied while keeping the partial pressures of all other species ($p_{j \neq i}$) constant.

The "degree of rate control" for step i ($X_{RC,i}$) was calculated using Campbell's theory[45-47] as,

$$X_{RC,i} = \frac{k_i}{r} \left( \frac{\delta r}{\delta k_i} \right)_{K_i, k_{j \neq i}}$$

where the equilibrium constant for step i ($K_i$) and all other rate constants ($k_{j \neq i}$) were held constant.

## 3. RESULTS AND DISCUSSION

### 3.1. *Ab initio* thermodynamic analysis for catalyst characterization.

We started the exploration for an appropriate catalyst model by investigating the most favorable edge sites of the BNNRs for $O_2$ adsorption using DFT and constrained thermodynamic analysis. All bare BNNRs studied possess the same number of atoms (128 atoms). As a result, comparisons can be made between the relative stability of these BNNRs before and after edge passivation with oxygen. Herein, we chose the dissociative adsorption of $O_2$ on the edge sites as suggested by Li et al.[29] The relaxed geometry of the fully oxygen passivated armBNNR (O@armBNNR), zzBNNR (O@zzBNNR) and mzzBNNR (O@mzzBNNR) are shown in Figures 1(e-g). $O_2$ was found to prefer molecular adsorption on the armBNNR edge, which agrees with the hypothesis of Grant et al.[14] and the findings of Li et al.[29] regarding the molecular oxygen adsorption on the armchair edge. The N-edge of zzBNNR favors the dissociative adsorption, while molecular adsorption of $O_2$ takes place on the B-edge. The dissociative adsorption of $O_2$ was found to be preferred on both edges of the mzzBNNR.
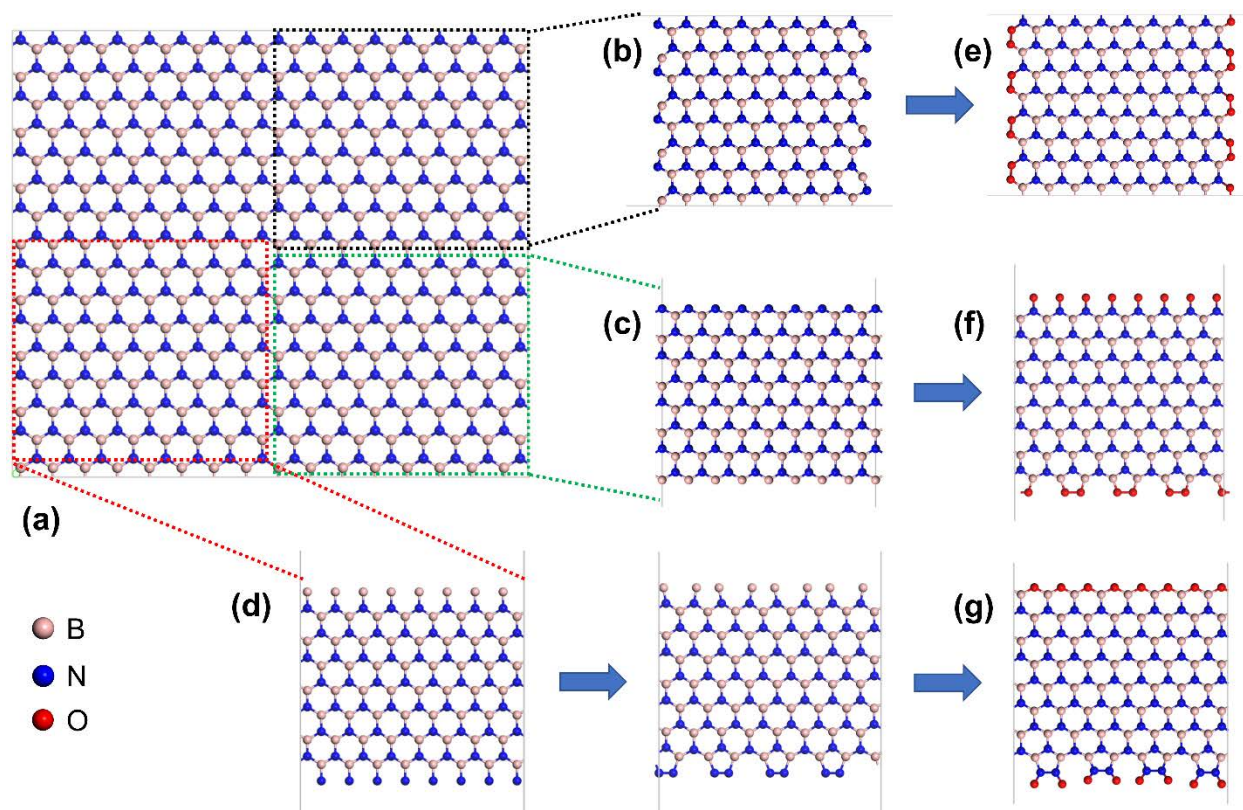
**Figure 1:** (a) Optimized structure of 16×16 orthorhombic 2D supercell of h-BN. The ribbon unit cell modeled from the 2D supercell is denoted by a black, green, and red dashed box for armBNNR, zzBNNR, and mzzBNNR, respectively. (b)-(c) Optimized structures of the bare unit cell of (b) armBNNR and (c) zzBNNR. (d) Unit cell of bare mzzBNNR before (left) and after (right) optimization. (e)-(g) Optimized structures of fully O passivated (e) O@armBNNR, (f) O@zzBNNR, and (g) O@mzzBNNR.

The results suggest that the mzzBNNR and zzBNNR are less stable compared to the armBNNR in bare form and the stability order was found to be armBNNR > zzBNNR > mzzBNNR, as shown in Figure 2(a) for zero O passivation. In order to understand the relative stabilities of the oxygen adsorbed edge sites, the adsorption Gibbs free energy ($\Delta G_{ads}$), was calculated using equation (**1**) with reference to the most stable bare form of BNNR, i.e., armchair BNNR, by varying the number of adsorbed O atoms on the edges of all three BNNRs and the results are plotted in Figure 2(a). While $\Delta G_{ads}$ does not seem to vary much with increasing number of O atoms on the armBNNR, a large variation of $\Delta G_{ads}$ was observed on the other two BNNRs.

After full O passivation, mzzBNNR becomes the most stable structure and the stability order

reverses to O@mzzBNNR > O@zzBNNR > O@armBNNR. This trend implies that the least

stable bare BN edge can eventually become the most stable BN edge after oxygen passivation

under reaction conditions. The decrease in free energy observed with increasing number of O

atoms on the three BNNRs clearly indicates that the BN edges are preferred to be O passivated

under ODHP reaction conditions.

To understand the process of O passivation at different edges of the BNNRs considered in

this study, the fully relaxed structures of each nanoribbon are shown with different numbers of O

atoms, 4O, 12O, and 14O in Figures 2(c)-2(k). O passivation starting from either edge of the

armBNNR will produce the same structure, but it can be different for the zzBNNR and mzzBNNR

as they possess two different edges, namely, a B-edge and a N-edge. Performed calculations

revealed that the adsorption of O atoms that start from the B-edge are energetically more favorable

than the corresponding adsorption on the N-edge for both the zzBNNR and mzzBNNR as shown

in Figure S1 of the Supporting Information. Hence, in the present work we considered O adsorption

starting from the B-edge for the *ab initio* thermodynamic analysis as shown in Figure 2. Figure

2(a) further reveals that the oxygen passivated armBNNR is still the most stable structure when

the number of adsorbed O atoms on all the BNNRs is below 6, but the stability of O@mzzBNNR

increases dramatically when the edges become passivated with more O atoms. Thus, BN edge

sites, similar to O@mzzBNNRs at high O passivation, likely exist under experimental reaction

conditions and might be a relevant active site for the ODHP reaction. Moreover, the variation of

$\Delta G_{ads}$ for O@mzzBNNR becomes small only when the number of adsorbed O atoms on the edge

is close to full passivation (nO > 12, Fig. 2b) suggesting that every five-membered ring on the N-

edge of O@mzzBNNR will have at least one adsorbed O atom under ODHP reaction conditions

as shown in Figure 2(j).  A closer look at the $\Delta G_{ads}$ variation of O@mzzBNNR (Fig. 2b) suggests that the structure with 12 adsorbed O atoms (here after referred as BNNR12O) is the most stable structure and a small increase in $\Delta G_{ads}$ was observed when more O atoms are added to this edge. Since the energy differences between BNNR12O and the ribbons thereafter with higher O passivation were found to be very small, any of these O adsorbed BNNR structures can be chosen as the initial catalyst model for the ODHP reaction (assuming that a redox cycle is possible between the structures having a difference in the number of O atoms of two and the initial catalyst can be regenerated from the other one through $O_2$ adsorption only with a small free energy penalty).

In order to further validate the stability of the potential O@mzzBNNR catalyst, we performed a constrained thermodynamic analysis for desorption of NO, $N_2O$ and $N_2$ gas molecules from the catalyst structure. The desorption of one $N_2$ molecule was considered through the removal of two edge N atoms from the bare five-membered ring of BNNR11O, while for $N_2O$ desorption removal of two edge N atoms with one O passivated at the edge five-membered ring from BNNR12O (Figure 2(j)) was considered. Similarly, removal of two N atoms with two O passivation atoms at the edge five-membered ring (having a $N_2O_2$ like composition) from BNNR13O, leading to desorption of two NO molecules, was studied. The free energies for desorption of these gas molecules were calculated at a temperature of 800 K using the same reference as before and are plotted in Figure 2(b). The partial pressure of $N_2$ gas was set to 0.55 atm which is consistent with the experimental gas concentration ratio of 3:6:11 of $O_2$:$C_3H_8$:$N_2$.[19] For the partial pressure of $N_2O$ and NO, we used a relatively low pressure of 0.001 atm to study the catalyst stability in presence of trace amounts of these molecules. Figure 2(b) reveals that the desorption of NO from BNNR13O, $N_2O$ from BNNR12O, and $N_2$ from BNNR11O yield structures that are 3.2 eV, 2.7 eV and 1.3 eV less stability than the parent nanoribbon, respectively, indicating

high stability of the considered catalysts. Based on our constrained thermodynamic analysis, $N_2$ desorption seems less energy demanding relative to NO and $N_2O$ desorption, however, it should be kept in mind that such desorption occurs through an energy barrier. In section 3.2, we discuss the pathway and energy barrier for $N_2$ desorption from the catalyst at practical reaction conditions.

In order to also explore the possibility of B loss, we performed a constrained thermodynamic analysis for removal of the oxygen passivated B edge from BNNR12O as a one-dimensional (1D) BO chain. We considered such 1D BO species as a precursor which can generate more stable bulk-like $B_2O_3$ species by reacting with oxygen molecules. The free energies for the B loss was calculated at a temperature of 800 K and compared with $N_2$, NO and $N_2O$ desorption from the considered catalysts and shown in Figure S10 of the Supporting Information. The optimized structures of the 1D BO, nanoribbon after BO removal (12O-$B_2O_3$), fully oxygen passivated nanoribbon after BO removal (O@12O-$B_2O_3$), and the unit cell of bulk $B_2O_3$ are shown in the same figure. Figure S10 reveals that the removal of edge BO from BNNR12O yields a nanoribbon with an additional N edge which is much less stable than the parent nanoribbon. Although oxygen passivation at this new N edge can improve the stability to some extent, it is still 7.6 eV uphill in energy relative to BNNR12O. Thus, B loss leading to the formation of bulk-like $B_2O_3$ species is thermodynamically uphill and hardly occurs.
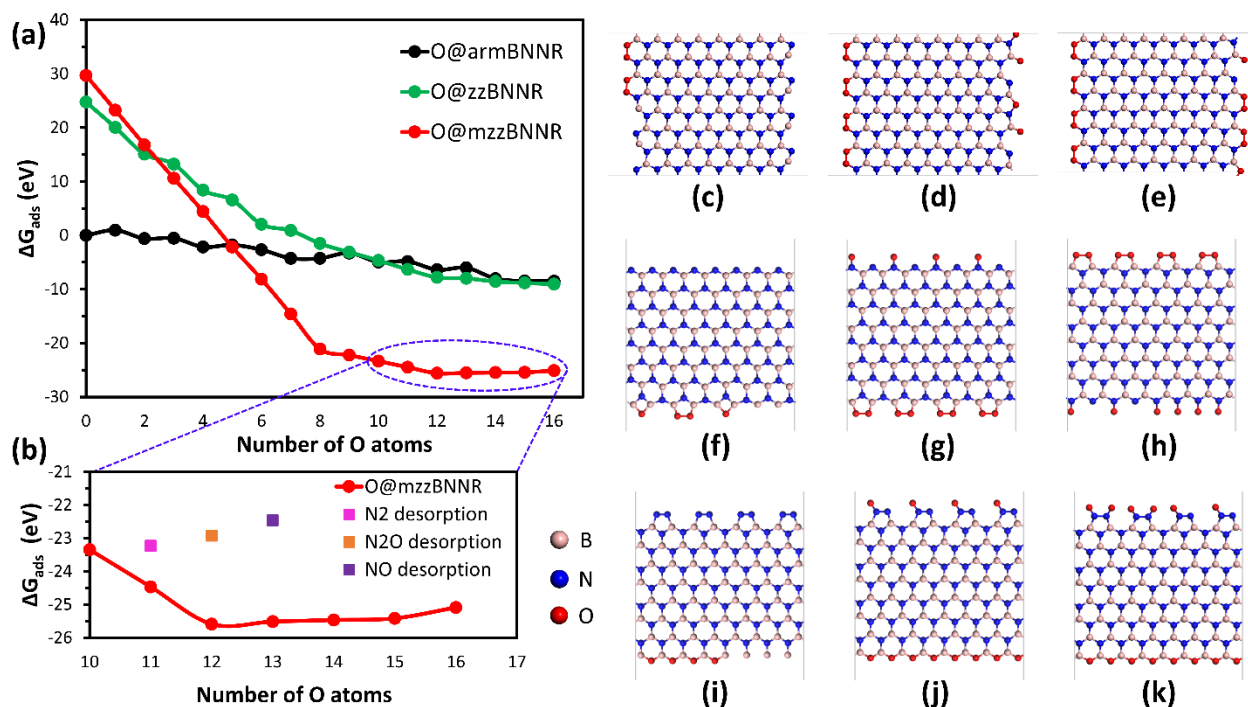
**Figure 2:** (a) Gibbs free energy ($\Delta G_{ads}$) variation with O passivation on the edges of the three BNNRs. (b) Close view of $\Delta G_{ads}$ variation with large number of adsorbed O atoms on the mzzBNNR edge. Color codes are shown in the corresponding insets. All free energies are calculated with reference to the energy of the optimized unit cell of bare armchair BNNR at T = 800 K and $P_{O_2}$ = 0.15 atm. $P_{N_2}$ = 0.55 atm, $P_{N_2O}$ = 0.001 atm, and $P_{NO}$ = 0.001 atm. (c) – (k) Optimized structures of 4O, 12O, and 14O passivated O@armBNNR (c-e), O@zzBNNR (f-g), and O@mzzBNNR (i-k), respectively.

## 3.2. Reaction Pathways of the ODHP at oxygen passivated mzzBNNRs

The *ab initio* thermodynamic analysis discussed above suggests that the BNNR edges remain oxygen passivated under ODHP reaction conditions, and that the O adsorbed mzzBNNR is the most stable structure under experimental reaction conditions. In order to identify a favorable site on this O@mzzBNNR that can activate propane, the BNNR14O structure was initially chosen (envisioning a catalytic cycle between BNNR14O and BNNR12O – also called Path I) and various possible intermediate structures were calculated for the first C-H cleavage of $C_3H_8$. The relaxed structures of fifteen different possible configurations of first H abstraction from $C_3H_8$ (namely, P1 to P15) on different sites of BNNR14O edges are shown in Figure S2 and the corresponding relative (free) energies are tabulated in Table S1 of the Supporting Information. All relative (free)

16

energies discussed in the mechanistic investigation are calculated with reference to the sum of the energies of BNNR14O, and the reactant gas molecules, $C_3H_8$ and $O_2$. The experimental reaction conditions[14, 15] of T = 800 K, $P_{C_3H_8} = 0.3$ atm, and $P_{O_2} = 0.15$ atm were used to calculate the relative free energies of intermediates and transition states involved in the mechanism. The large positive relative energy and free energy values observed for the configurations P1 ($\Delta G = 7.21$ eV) and P2 ($\Delta G = 4.18$ eV), where the H abstraction occurs on the B-edge of BNNR14O, clearly indicate that this mechanism on the B-edge of the BNNR14O is not active for H abstraction from $C_3H_8$, since it requires breaking of the B–O–B ring structure to initiate the ODHP reaction. In addition, we investigated the heterolytic C-H activation mechanism over a B-O pair to form a propyl bonded to B, and a hydrogen bonded to an adjacent O (Figure S2(c) and P3 in Table S1) on the oxygen passivated B-edge of BNNR14O similar to the ODHP mechanism proposed by Zhang et al.[48] over $B_2O_3$. Again, we found a large positive relative free energy value of 2.58 eV. Next, Lu et al. proposed that a hydroxyl group on B, created by cleavage of the B-O bond in boron oxide through water adsorption, can react with $O_2$ to form a peroxo species that is active for C-H abstraction in the ODHP reaction over mesoporous silica-supported boron oxide catalysts.[49] We have explored the relative stability of similar species that can possibly form through water adsorption on the oxygen passivated B-edge of BNNR14O (Figure S2(d)), leading eventually to a peroxo species (Figure S2(e)) after reaction with oxygen for C-H abstraction. We observed a large positive relative free energy value of 3.08 eV for this peroxo species (P5) as tabulated in Table S1. Therefore, we conclude that the O passivated B-edge of the mzzBNNR is not the active site for the ODHP reaction. Instead, all the configurations on the N-edge (P6 to P15) display a favorable first H abstraction from $C_3H_8$ with negative $\Delta E$ values and relatively small positive $\Delta G$ values as shown in Table S1 of the Supporting Information. Thus, these calculations indicate that the O passivated

mzzBNNR N-edge can be the active site for the ODHP reaction and we designate this active site as a $N_2O$ or $NO_x$ site. The most stable configuration on the N-edge was found to be P14 (Figure S2(n)) with $\Delta E = -1.3$ eV and $\Delta G = 0.2$ eV, where the secondary H of $C_3H_8$ was abstracted by one bare N atom and the propyl group ($C_3H_7$) binds with the adjacent O. These N and O atoms are referred to as $N_{e1}$ and $O_{e1}$, respectively, as shown in Figure S2(n). Furthermore, the relative stabilities of the different configurations of the first H abstraction from $C_3H_8$ on other O@mzzBNNRs with different number of O atoms such as BNNR11O, BNNR12O, BNNR13O and BNNR15O have been investigated, and were found to have a configuration similar to P14 on BNNR14O, which is the most stable configuration on all the BNNRs. Therefore, in the proposed reaction mechanism for the ODHP, the P14 configuration was considered as the first H abstracted intermediate structure (IM2, Figure 3) on the catalyst BNNR14O. The proposed mechanism of the ODHP reaction on the chosen O@mzzBNNR catalyst follows a pathway in which $C_3H_8$ first binds and reacts with the catalyst and then desorbs as $C_3H_6$ leaving two H atoms on the catalyst. The H atoms can undergo rearrangement through the edge to produce $H_2O$ and create an oxygen vacancy on the catalyst. Subsequently, a similar pathway for the reaction of a second $C_3H_8$, which leads to the formation of two oxygen vacancies on the BNNR edge, was considered. These vacancies can be replenished by dissociative adsorption of $O_2$. The overall reaction of the ODHP on an O@mzzBNNR catalyst can be written as,

$$O_n@mzzBNNR + 2C_3H_8 \rightarrow O_{n-2}@mzzBNNR + 2C_3H_6 + 2H_2O \qquad (4)$$

$$O_{n-2}@mzzBNNR + O_2 \rightarrow O_n@mzzBNNR \qquad (5)$$

A schematic representation of three different possible catalytic cycles, starting with a different number of surface oxygen atoms (14O to 12O; 13O to 11O; and 12O to 10O), considered in the present work is shown in Figure 3. We note that the relative stability of all of these structures in

18

Catalysis Science & Technology

the catalytic cycles are similar (see Figure 2), that all pathways are coupled, and that only a full microkinetic model as developed later in this section can determine the most dominant reaction cycle.
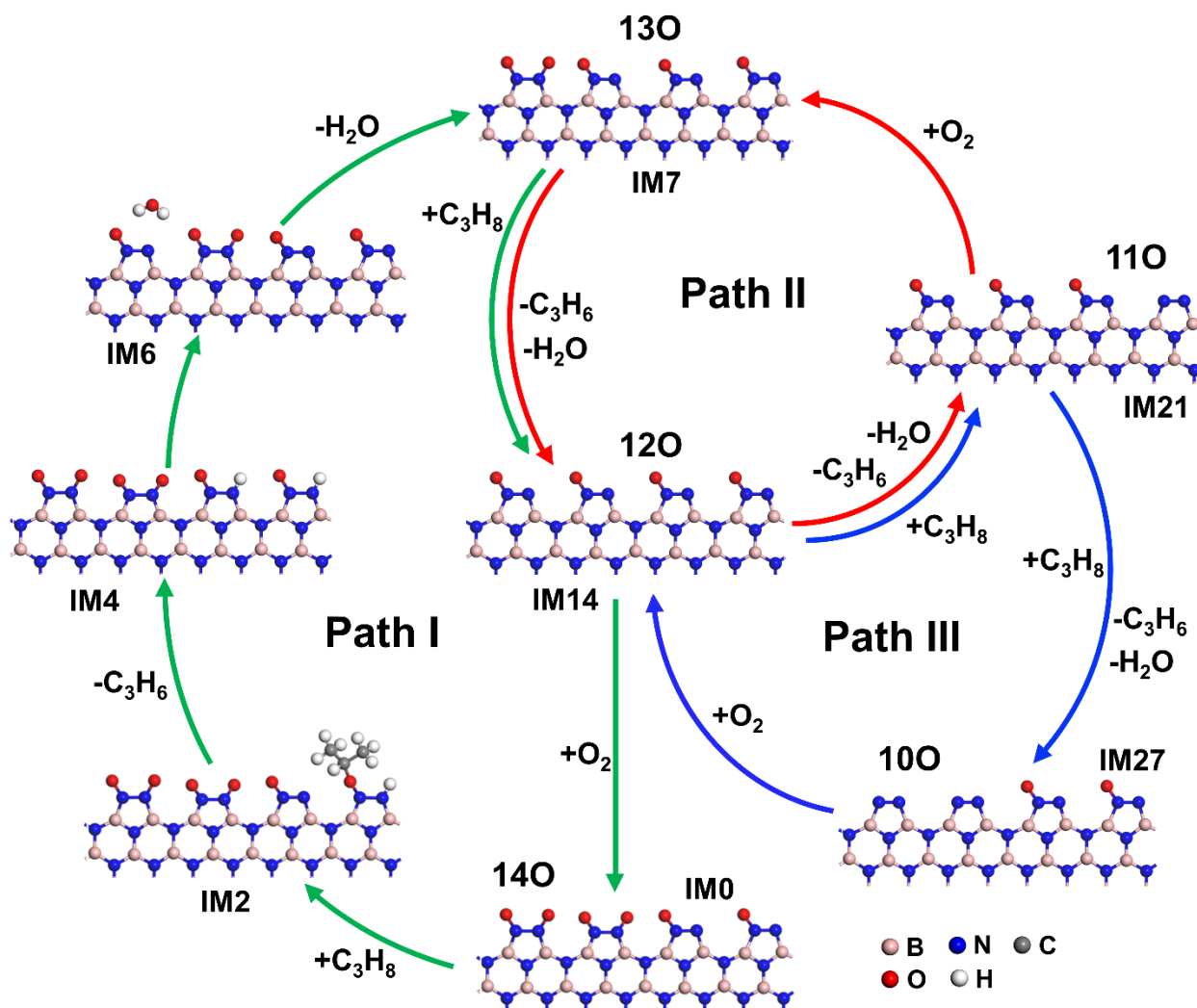


**Figure 3:** Schematic representation of three different reaction cycles of the ODHP reaction on the chosen O@mzzBNNR catalyst. The 14O to 12O cycle (also called Path I), the 13O to 11O cycle (also called Path II), and the 12O to 10O cycle (also called Path III) are indicated with green, red, and blue arrows, respectively. Somewhat more mechanistic details are shown for Path I that are also present in the other pathways.
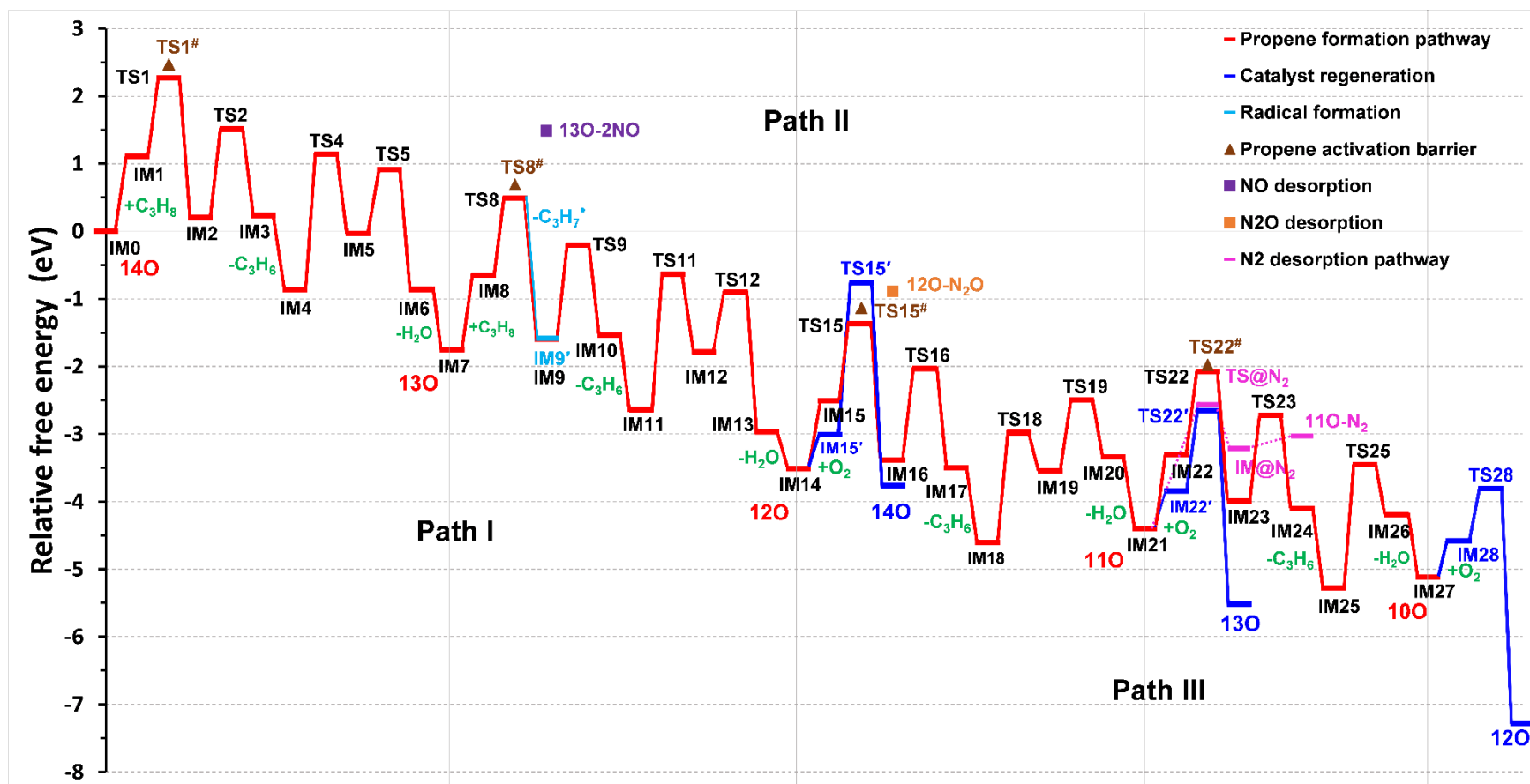
**Figure 4:** Free energy profiles for three different (coupled) catalytic cycles (Path I: 14O to 12O; Path II: 13O to 11O; and Path III: 12O to 10O) of the ODHP reaction on the O@mzzBNNR catalysts. Color code of different parts of the pathways are shown in the inset. All free energies are calculated with reference to the sum of the energies of BNNR14O and the reactant gas molecules, at T = 800 K, $P_{C_3H_8}$ = 0.3 atm, $P_{O_2}$ = 0.15 atm, $P_{C_3H_6}$ = 0.3 atm, $P_{H_2O}$ = 0.3 atm, $P_{C_3H_7^\bullet}$ = 0.3 atm, $P_{N_2}$ = 0.55 atm, $P_{N_2O}$ = 0.001 atm, and $P_{NO}$ = 0.001 atm.

Figure 4 illustrates the calculated relative Gibbs free energy profiles for all three (coupled)

reaction pathways at a representative temperature of 800 K. The corresponding energy profile is

shown in Figure S3 of the Supporting Information. For Path I (see Figure 3), the ODHP reaction

starts with the weak adsorption ($\Delta E = -0.01$ eV) of a $C_3H_8$ molecule (IM1) on the initially chosen

catalyst edge (BNNR14O, IM0), followed by an H abstraction from the secondary carbon of $C_3H_8$

leading to a stable propyl intermediate (IM2). For the second H abstraction from the stable propyl

intermediate, one H from either methyl group is abstracted by the bare $N_{e2}$ atom leading to an

intermediate (IM3) with adsorbed $C_3H_6$. Desorption of a $C_3H_6$ molecule leaves two H atoms on

the ribbon (IM4). In the following steps, the remaining two H atoms on IM4 can rearrange through

the edge oxygen atoms and the two neighboring OH groups react to produce one $H_2O$ molecule

and an O vacancy on the ribbon (IM6). Different possible H rearrangement pathways were

examined, and the optimized structures of these intermediates together with the relative free

energies of the intermediates and TSs involved are shown in Figure S4 of the Supporting

Information. The highest energy barrier from the H rearrangement network (Figure S4) constitutes

the effective energy barrier for the H rearrangement process (TS4) and is shown in the free energy

diagram (Figure 4). Next, desorption of $H_2O$ from IM6 leads to a nanoribbon with one less oxygen

(BNNR13O, IM7). BNNR13O can again react with another $C_3H_8$ molecule to produce a second

set of products, $C_3H_6$ and $H_2O$, while creating a second oxygen vacancy in the nanoribbon

(BNNR12O, IM14) following a similar reaction sequence as mentioned above. Now, the initial

catalyst (BNNR14O) can be regenerated by the dissociation of an $O_2$ molecule on BNNR12O

(IM14) which completes the 14O→12O→14O catalytic cycle of Path I. Our calculations revealed

that this $O_2$ dissociation process (TS15′) requires a high activation barrier of 2.76 eV. In Path II

and Path III, BNNR12O (IM14) can react further with another $C_3H_8$ molecule through a much

21

lower barrier (TS15) than TS15′ and eventually produce BNNR11O (IM21) through desorption of a $C_3H_6$ and a $H_2O$ molecule, in a similar mechanism to that of 14O→13O or 13O→12O. Next, adsorption and dissociation of $O_2$ on IM21 (BNNR11O) was considered to regenerative the BNNR13O (IM7) active site and close the catalytic cycle of Path II which requires an activation barrier of 1.74 eV (TS22′) which is more than 1 eV lower than the $O_2$ dissociation process of Path I. Further reaction of BNNR11O (IM21) with $C_3H_8$ to produce BNNR10O (IM27) was also considered and is called Path III in Figure 3 and 4. However, the free energy barrier for the propane activation on BNNR11O (TS22) was found to be 0.58 eV higher than the barrier for $O_2$ dissociation (TS22′, Fig.4). A closer look at the free energy diagram involving all 3 pathways (Path I, II, and III) (Fig. 4) suggests that the cycle starting from BNNR13O (Path II) possesses lower activation barriers and thus, is likely more favorable over the other two cycles. The optimized structures of the intermediates involved in Path II of the ODHP reaction starting from the BNNR13O (IM7) catalyst are provided in Figure 5. The corresponding TS structures are shown in Figure S5 of the Supporting Information. Different possible H rearrangement pathways (from IM11 to IM12) were examined and the optimized structures of these intermediates together with the relative free energies of the intermediates and TSs involved are shown in Figure S6 of the Supporting Information. The highest energy barrier was chosen from the H rearrangement network (Figure S6) as the effective energy barrier for the H rearrangement process (TS11) and is shown in the free energy diagram (Figure 4) similar to what was done in the BNNR14O case (Path I).
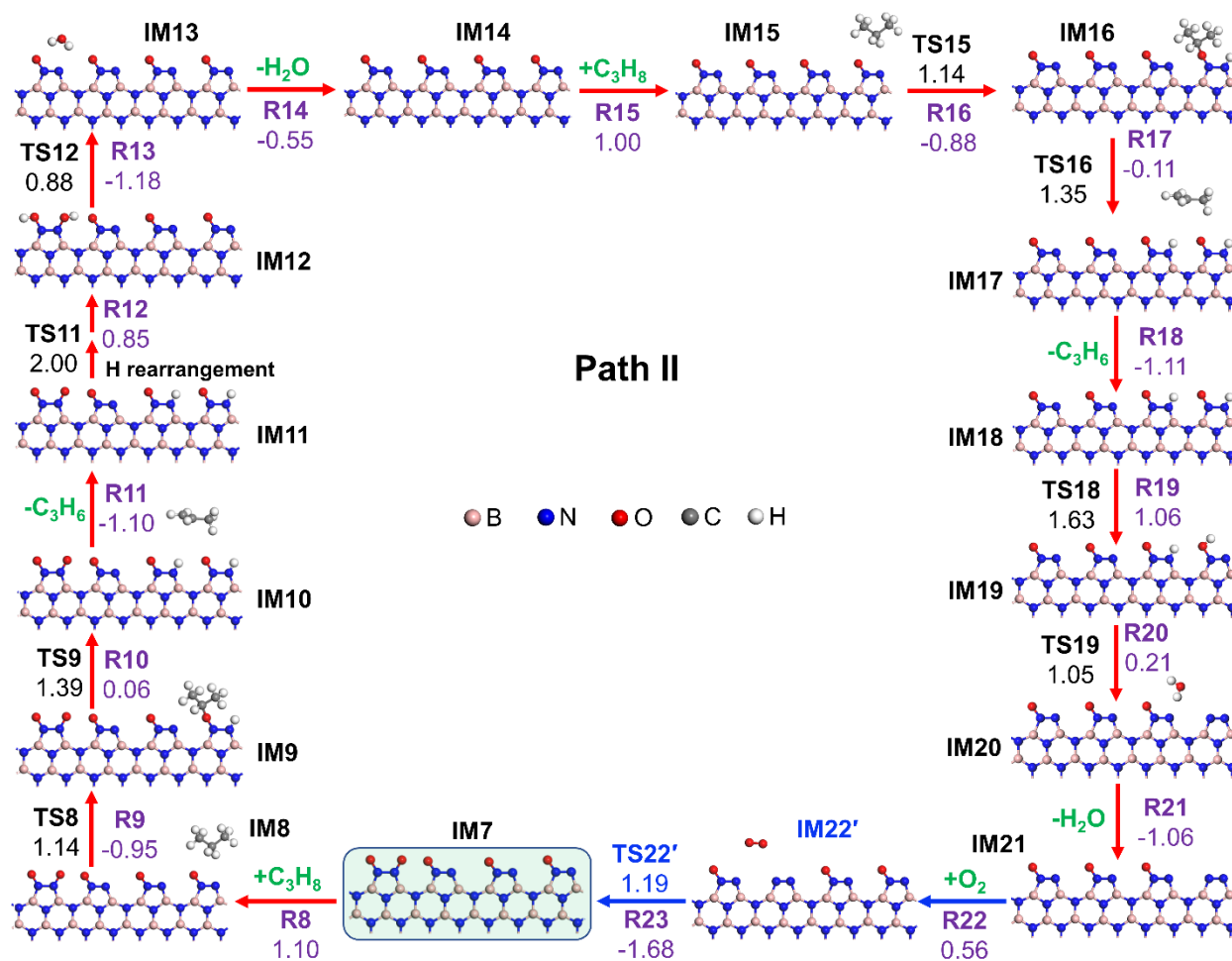
**Figure 5:** Reaction network of various ODHP reaction steps in the catalytically most relevant cycle, Path II, that starts on the BNNR13O catalyst structure (IM7, marked by light green box). Color code of the pathways is consistent with Figure 4. The reaction free energies (purple) and free energy barriers (black) of each elementary step are shown in eV. T = 800 K, $P_{C_3H_8}$ = 0.3 atm, $P_{O_2}$ = 0.15 atm, $P_{C_3H_6}$ = 0.3 atm, and $P_{H_2O}$ = 0.3 atm.

In addition to the ODHP pathways discussed above, we also examined the feasibility of a gas phase ODHP reaction initiated by the BN catalyst as experimentally speculated by Venegas et al.[22] In the surface catalyzed cycle, the first C-H cleavage of adsorbed $C_3H_8$ transfers an H atom to the bare N atom of the BNNR edge and the remaining propyl group is transferred to the O atom adsorbed on the neighboring N atom. Our NEB calculations for this process and the optimized TS structure (TS8 in Figure 6) suggest that this process initially forms a $C_3H_7^\bullet$ radical after H-transfer which then moves to the neighboring surface O site in a barrier-less downhill process.

Alternatively, the $C_3H_7^{\bullet}$ radical can also desorb as a gas species and participate in a gas phase ODHP reaction. The concept of such a single TS leading to two different product states is well established.[50] To check the feasibility of such a gas phase radical generation, the relative free energy for the $C_3H_7^{\bullet}$ radical desorption process at 800 K (shown in Figure 4 as IM9′) was calculated. Results showed that the free energies of IM9 (-1.60 eV) and IM9′ (-1.58 eV) are nearly the same. Thus, at 800 K, the generation of a gas phase $C_3H_7^{\bullet}$ radical seems to be equally likely to that of the surface adsorbed stable intermediate. Although, the extent of gas phase radical formation will depend on the applied temperature and partial pressure of $C_3H_8$, it can be concluded that the proposed $N_2O/NO_x$-type active sites on the BN edge can also generate $C_3H_7^{\bullet}$, which in turn can trigger gas phase reactions for the ODHP as experimentally speculated.[22] Although, a full microkinetic analysis of these gas phase reaction is outside the scope of the present work, we can at least speculate that the presence of such gas phase mechanism may be the reason for the presence of other cracking byproducts found under experimental conditions.

In addition to propane activation, high selectivity to propene is one of the key features of the BN catalyst for the ODHP. In other words, if the proposed $N_2O/NO_x$ active site is relevant for the experimental system, it has to be selective for propane activation relative to further activation of propene. Although, a full microkinetic analysis of all propene activation steps is outside the scope of the present work, we have calculated the barrier for propene activation over the considered catalysts shown in Figure 4 (shown in rust color triangles and designated with superscript #). The relative (free) energy barriers for propene activation over the proposed $N_2O/NO_x$ active sites are summarized and compared with corresponding propane activation barriers in Table S2 of the Supporting Information. We found that over all the catalysts, the barrier for propene activation is about 0.2 eV higher than the corresponding propane activation (except for BNNR11O, where it is

0.1 eV higher). Thus, at similar propane ($C_3H_8$) and propene ($C_3H_6$) partial pressures, the selectivity to propene (versus propene activation products such as $C_2H_4$ and $CO_x$) can be estimated from $\frac{r_{propene}^{consumption}}{r_{propene}^{production}} = e^{\left(\frac{-\left(\Delta G_{C3H6}^{TS} - \Delta G_{C3H8}^{TS}\right)}{k_B T}\right)}$, where $\Delta G_{C3H6}^{TS} - \Delta G_{C3H8}^{TS}$ is the difference between the free energy barriers of propene and propane activation, respectively. For a free energy barrier difference of 0.2 eV, we obtain a propene selectivity of ~95% at 800 K. This indicates that the considered $N_2O/NO_x$ active site on the BN edge is indeed selective for the propene production. As a word of caution, we note that if the difference in activation barrier is only 0.1 eV (which is certainly within the uncertainty range of DFT), then the predicted propene selectivity at equal partial pressures of propane and propene would only be ~80%. In other words, it is very challenging to accurately quantify all reaction products from the $N_2O/NO_x$ type active site. Also, the proposed catalyst is expected to generate $C_3H_7\bullet$ radicals that can trigger gas phase reactions as experimentally speculated and that can dissociate to into the experimentally observed $C_2H_4$ and $CH_3\bullet$ radical.

To understand why our proposed $N_2O/NO_x$ active site is active for H abstraction in the ODHP reaction, it is important to note that the $N_2O/NO_x$ active site consists of a bent $N_2O$ like structure. Due to the bent nature (gas phase $N_2O$ is linear), we observe charge separation within the active site and charge transfer during abstraction of the H atom from propane during catalysis. Specifically, Figure S11 of the Supporting Information illustrates results from a Bader charge analysis of the atoms of the active site of BNNR13O (IM7) during catalysis. Clearly, the distant N and O-atoms of the bent $N_2O$ active site are highly negatively charged, polarizing propane. Furthermore, the active site can accept more electrons from the dissociating propane in the transition state, TS8, and the product state, IM9, illustrating the ability of the active site to perform redox chemistry.

25

As already mentioned earlier, we are also interested in the stability of the proposed $N_2O/NO_x$ sites with regards to desorption of gas-phase molecules. Thus, the relative free energies for desorption of two NO molecules from 13O (IM7), one $N_2O$ molecule from 12O (IM14) and one $N_2$ molecule from 11O (IM21) were computed at 800 K using the same energy reference of our proposed reaction network (see Figure 4). The partial pressures of $N_2$, $N_2O$ and NO were set to 0.55 atm, 0.001 atm and 0.001 atm, respectively, as discussed in section 3.1. Figure 4 shows that the final structure after removal of two NO molecules from 13O (IM7), designated as 13O-2NO and shown in purple square in Figure 4, is 1 eV higher in free energy than the propane activation barrier (TS8) on 13O. Similarly, the structure after one molecule of $N_2O$ desorption from 12O (IM14), designated as 12O-$N_2O$ and shown in orange square in Figure 4, is 0.5 eV higher than the propane activation barrier (TS15) on the corresponding catalyst. Also, desorption of one molecule $N_2$ from 11O (IM21) produces a structure (designated as 11O-$N_2$ in Figure 4) that is 1.3 eV less stable than 11O, but 0.4 eV lower in energy than the $O_2$ dissociation barrier (TS22′) on 11O. We note however that $N_2$ desorption also involves an energy barrier in which the edge N atoms of the bare five-membered ring of 11O are bonded to two different B atoms. Before desorption of these N atoms as a $N_2$ molecule, they first produce a high energy structure where $N_2$ is vertically bonded to one B atom (designated as IM@$N_2$ in Figure 4). The transition state to form IM@$N_2$ (designated TS@$N_2$ in Figure 4) is 0.1 eV higher in energy than the $O_2$ dissociation barrier (TS22′) on 11O. The optimized structures of the intermediates and TS involved in the $N_2$ desorption pathway are provided in Figure S7 and corresponding relative free energies and ZPE corrected energies are tabulated in Table S2 of the supporting information. Comparing the energy profile for $N_2$ desorption (shown as pink dotted line in Figure 4) form the bare edge five-membered ring of 11O to that of $O_2$ adsorption and dissociation at the same site (shown in blue solid line in

Figure 4), one can deduce that it is more likely that $O_2$ will bind and dissociate over 11O to reproduce 13O, rather than catalyst degradation through $N_2$ desorption. In other words, we conclude that the proposed $N_2O/NO_x$ active site does not favor its decomposition into the gas phase but rather reacts with propane to produce propene. Nevertheless, $N_2$ desorption is potentially a pathway for slow catalyst deactivation as observed experimentally and increasing the partial pressure of $N_2$ likely helps stabilizing the catalyst.
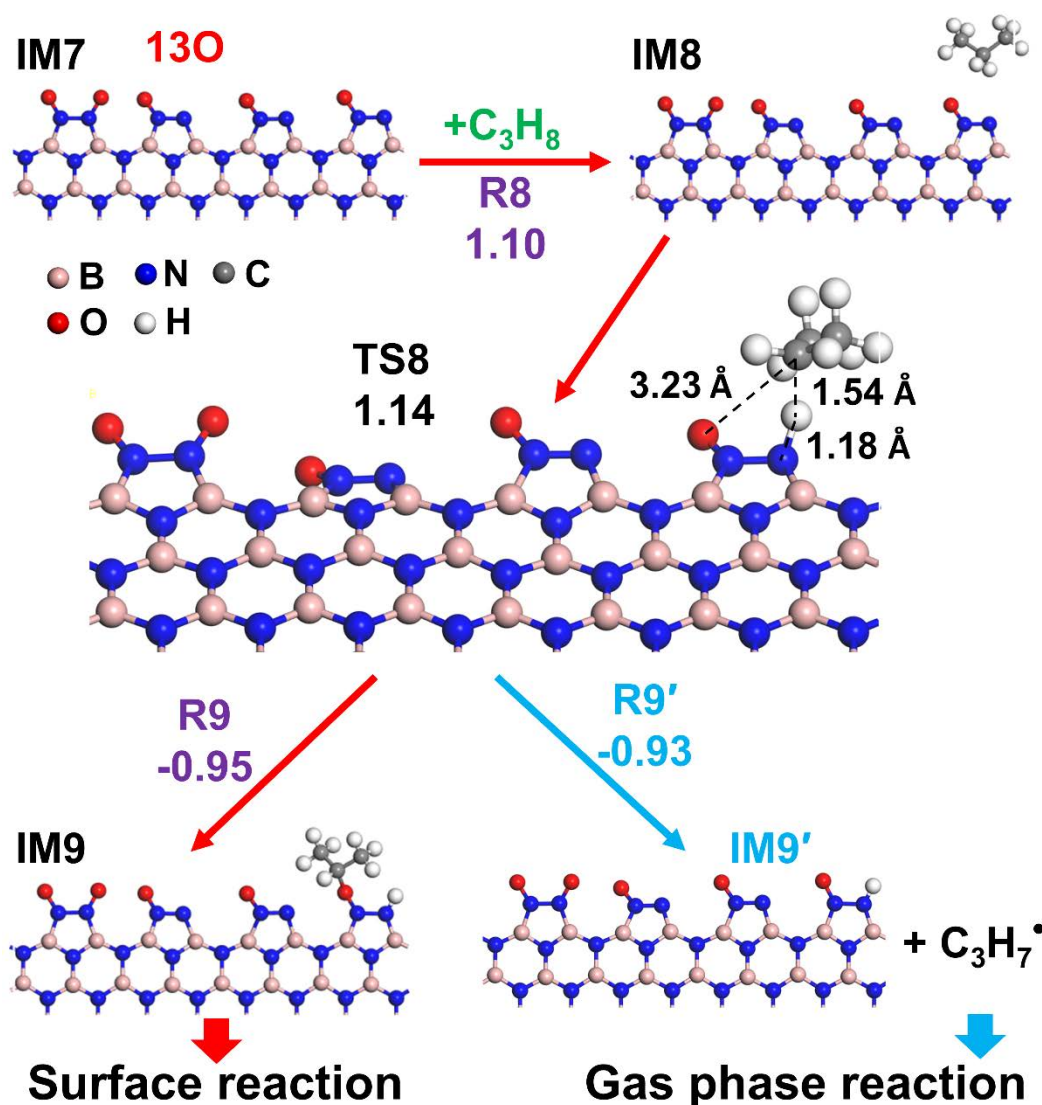
**Figure 6:** Schematic representation of propyl radical ($C_3H_7^{\bullet}$) formation from the TS of the first C-H cleavage of adsorbed $C_3H_8$ on the BNNR13O active site structure. The reaction free energies and free energy barriers of each elementary step are the same as those shown in Figure 5.

### 3.3. Insights from Microkinetic Modeling.

In order to better understand the relative rates of the different catalytic cycles and to calculate other kinetic parameters for the ODHP reaction on the mzzBNNR catalyst under experimental reaction conditions, we developed a microkinetic model based on the DFT data and harmonic transition state theory that involves all pathways, i.e., Path I, II, and III. All elementary steps of the proposed reaction network shown in Figure 3 and Figure 4 have been considered. In the microkinetic model, we used a temparature range from 723 K to 823 K and set the partial

28

pressures of the reactant gas molecules to $P_{C_3H_8} = 0.3$ atm and $P_{O_2} = 0.15$ atm to maintain

consistency with the experimental reaction conditions.[14, 15, 19]

　　　The results obtained from the microkinetic analysis of the overall reaction network are

summarized and compared with available experimental data in Table 1. The 33 elementary

reactions along with the ZPE corrected reaction energies and forward activation barriers are

summarized in Table S3 of the Supporting Information. The forward rate and equilibrium

constants for all the elementary reactions, and the surface coverages calculated at three different

temperatures (748 K, 798 K and 823 K) are summarized in Table S4 and Table S5 of the

Supporting Information, respectively. The overall turnover frequencies (TOFs) calculated in the

temperature range of 748 – 823 K are on the order of $10^{-2}$ s$^{-1}$ which suggest that the proposed

N$_2$O/NO$_x$-type active sites on the mzzBNNR catalyst can exhibit a high activity for the ODHP

reaction at these conditions. The individual reaction rates of the different reaction cycles predicted

from the microkinetic analysis of the overall network in the temperature range of 748 K to 823 K

are also tabulated in Table 1. These rates indicate that Path II, involving 13O and 11O, is the

dominant catalytic cycle for the overall ODHP activity of our proposed catalyst, which is

consistent with the free energy profile shown in Figure 4. The lower rates observed for the other

two cycles starting from 14O (Path I) and 12O (Path III) can be explained based on the stability of

these structures computed by *ab initio* thermodynamic calculations and shown in Figures 2(a) and

2(b). These plots show that the structure 12O, where every five-membered ring on the N-edge is

occupied by one O atom, is the most stable structure under ODHP reaction conditions and the

relative free energies do not change much when adding more O atoms to this structure. For a

catalytic cycle between 14O and 12O, the effective free energy barrier of the O$_2$ dissociation

process on 12O to regenerate 14O was found to be as high as 2.76 eV (Fig. 4) which leads to four

order of magnitude lower rates than the catalytic cycle starting from 13O. The $O_2$ dissociation process on the 11O structure, which leads to the 13O structure, exhibits a much lower activation barrier (1.74 eV), due to the highly favorable thermodynamic driving force for this reaction as shown in Fig. 2b. Although this process is both thermodynamically and kinetically even more favorable in Path III involving 12O and 10O, the forward process, i.e., the creation of each oxygen vacancy from 12O, is highly endergonic. The high endothermicity of the oxygen vacancy formation process in Path III results in an overall higher activation barrier for the second propane activation on 11O leading again to a lower ODHP reaction rate for this catalytic cycle.

**Table 1:** The turnover frequency (TOF), apparent activation energy ($E_{app}$), and reaction orders calculated from a microkinetic reactor analysis of the proposed overall ODHP reaction.

| Reaction pathway | TOF ($s^{-1}$) | | | $E_{app}$ (eV) | Rate-limiting step | Reaction order (T= 798 K) | |
|---|---|---|---|---|---|---|---|
| | 748 K | 798 K | 823 K | | | $C_3H_8$ | $O_2$ |
| Overall reaction | $1.4 \times 10^{-2}$ | $5.1 \times 10^{-2}$ | $8.8 \times 10^{-2}$ | 1.34 | 1st C-H cleavage of $C_3H_8$ on the catalyst | 0.9 | 0.0 |
| Path I: 14O to 12O cycle | $1.4 \times 10^{-6}$ | $6.3 \times 10^{-6}$ | $1.5 \times 10^{-5}$ | | | | |
| Path II: 13O to 11O cycle | $1.4 \times 10^{-2}$ | $5.1 \times 10^{-2}$ | $8.8 \times 10^{-2}$ | | | | |
| Path III: 12O to 10O cycle | $1.2 \times 10^{-6}$ | $1.1 \times 10^{-5}$ | $2.9 \times 10^{-5}$ | | | | |
| Experimental | | | | 2.62[a] 1.91[b] | Propane activation[c] | 2.0[a,c] | 0.5[c] |

[a]See ref 14. [b]See ref 15. [c]See ref 18.

A degree of rate control analysis[45-47] on the overall reaction network suggests that the first C-H cleavage of adsorbed $C_3H_8$ on the 13O structure is the rate controlling step of the overall reaction, which is consistent with the corresponding highest effective barrier (TS8) observed for Path II (13O→11O→13O cycle) in the free energy profile of Figure 4. This result agrees well with the exprimental prediction of Shi et al.[18] that the total rate of the ODHP reaction on the boron nitride catalyst is determined by the activation of propane. An observation that is based on the observation of a kinetic H/D isotopic effect of 1.4-1.5.  The next step in this study was to calculate the apparent activation barrier of 1.34 eV from the Arrhenius plot shown in Figure 7, which is somewhat smaller than the reported experimental barrier of 2.62 eV and 1.91 eV.[14, 15] Furthermore, our calculations predicted a near first-order dependence on $C_3H_8$ and zero-order dependence on $O_2$ (see Figure S8 of the Supporting Information) which also seems to disagree with the second-order dependence on $C_3H_8$ and half-order on $O_2$ reported by previous experimental studies.[14, 15, 18] It is worth mentioning though that the Microkinetic Reactor Analysis used in this current study involves only the elementary steps of ODHP reactions that occur on the BNNR edge. In the previous section, we discussed the possibility of gas phase $C_3H_7^\bullet$ radical generation, which can trigger a gas phase ODHP reaction at high temperatures as experimentally hypothesized. In fact, the same rate limiting step identified for the catalytic ODHP reaction is also responsible for the generation of the $C_3H_7^\bullet$ radical that could split into the experimentally observed $C_2H_4$ and $CH_3^\bullet$ radical.[48] Thus, we believe that the discrepancy in the reaction orders and apparent activation barrier between our current study and the experimental reports could originate from the occurrence of a gas phase ODHP reaction at high temperature in parallel to the surface catalyzed reaction considered here. We note that inclusion of a gas-phase reaction mechanism in our reaction model is beyond the scope of this study, given that such a coupled gas and solid phase model requires

knowledge of the gas phase volume relative to the number of active surface sites, and consideration of heat, mass, and momentum transfer specific for the experimental reactor and reaction conditions. We note however that gas phase reactions can be suppressed experimentally by heating the catalyst-support system under microwave (MW) irradiation. It is well established that for materials with good microwave absorption properties, large and stable temperature differences of approximately 50 K between a colder gas phase and a hot solid can be established, helping to avoid undesired gas phase reactions.[51, 52] Ramirez et al. have recently applied MW heating to increase the selectivity to propylene in the oxidative dehydrogenation of propane over SiC monolithic reactors coated with a VMgO catalyst, by avoiding undesired gas phase reactions.[52] We note that the microwave absorption properties of BN can be improved through suitable multilayer graphene/BN or BN/SiC nanoparticle hybrid formation.[53, 54] It is under these conditions that it would be very interested in knowing whether the experimentally determined kinetic parameters in the microwave reactor are closer to those predicted by us and thus, that they differ significantly from those measured in a conventional reactor.

Next, we note that another reason for the discrepancy in experimentally measured apparent activation barrier and reaction orders relative to our predicted data is the (in our opinion) high likelihood that the experimentally determined kinetic parameters include at least two material processes: (i) the catalysis on the active site and (ii) the creation of the active site. If the latter is a function of propane and oxygen concentration and temperature, e.g., more active sites are present at higher temperatures, then higher apparent activation barriers and reaction orders are measured than those corresponding to the catalytic cycle on the active sites that are determined by our models. In particular, we note that the very high apparent activation barrier of 2.62 eV measured by Grant et al.[14, 15] (which is nearly twice as large as the one predicted by us of 1.34 eV) can hardly

originate only from the catalytic cycle. Due to the entropy penalty of gas phase adsorption at 800 K, our computed effective free energy barrier is 2.24 eV (see Figure 4 and 5). In other words, even in the most favorable circumstances of no entropic penalty in the experimentally measured catalytic cycle, the active site measured by Grant et al. would be 0.38 eV or approximately a factor of 250 (at 800 K) less active than our identified $N_2O/NO_x$ site if the measurement would exclusively involve processes in the catalytic cycle. Such a rate would likely be too low for a practical catalyst and it is more likely that the experimentally measured kinetic parameters contain in addition to the catalytic cycle, processes that are involved in the creation of the active site. Thus, it is not surprising that our computationally predicted kinetic parameters do not agree with those measured. We note however that our predicted selectivity agrees well with the measurements and that selectivity is only a function of the reaction mechanism on the surface (and in the gas phase).
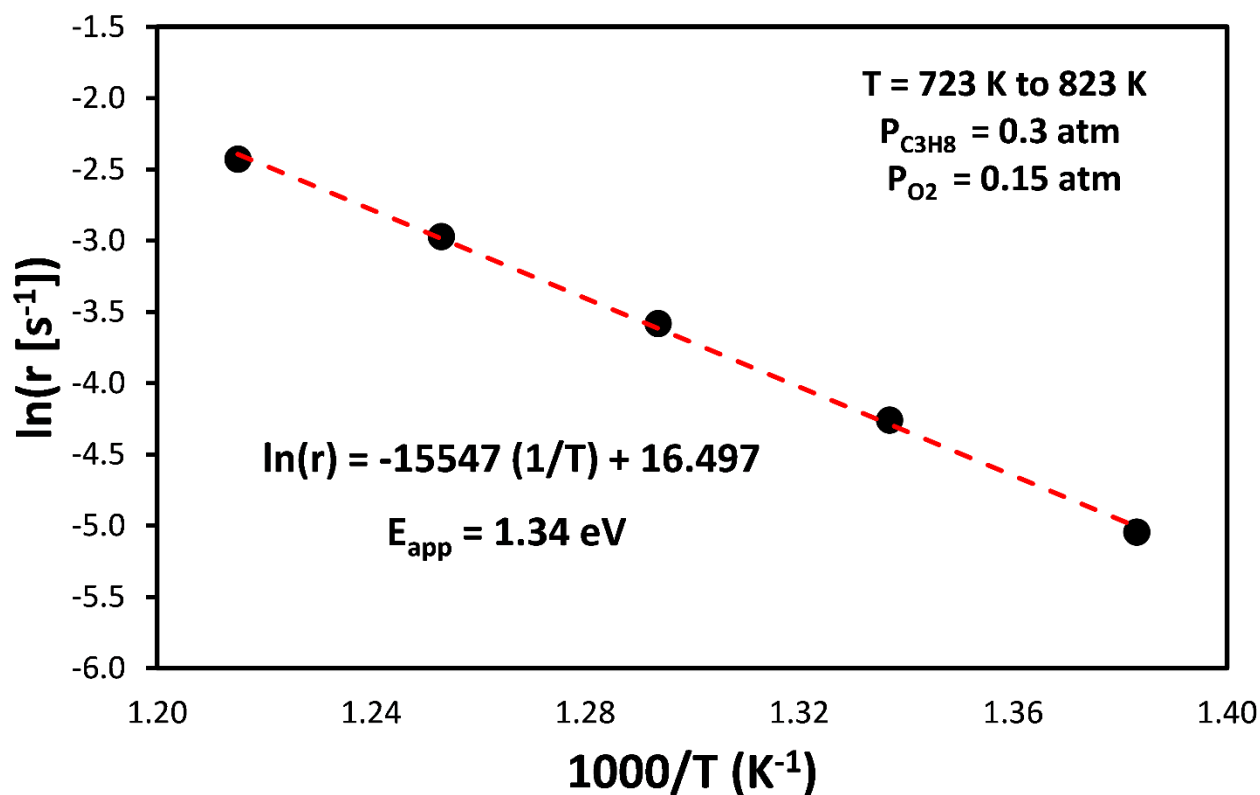
**Figure 7:** Arrhenius plot for the overall reaction, revealing an apparent activation energy of 1.34 eV in a temperature range of 723 to 823 K, and $P_{C_3H_8} = 0.3$ atm, $P_{O_2} = 0.15$ atm.

Finally, we note here that we used standard DFT with the PBE functional to explore the ODHP reaction over a $N_2O/NO_x$-type active site. To examine the effect of van der Waals interactions and a different DFT functional on the ODHP reaction, a full optimization with SCAN+rVV10[36, 37] and PBE-D3 functional were carried out for the most critical elementary steps of Path I (see Figure 4), i.e., the first C-H cleavage of $C_3H_8$ on the catalyst and direct dissociation of $O_2$ over BNNR12O to reproduce the catalyst BNNR14O. The calculated results using PBE-D3 and SCAN+rvv10 functionals are compared with the PBE results in Table S6 of the Supporting Information. Both the PBE-D3 and SCAN+rvv10 predicted very similar structures for the IMs and TSs (as shown by the bond distances involved in the TSs in Table S6 and the fully optimized

structures in Figure S9 of the Supporting Information) for these elementary steps as found by the PBE functional. The data in Table S6 suggest that SCAN+rvv10 predict slightly higher reaction barriers (~0.2 eV) than PBE while at the same time slightly destabilizing (~0.1 eV) the most stable intermediate (12O) of that cycle. In contrast, fully optimized PBE-D3 calculations predict a somewhat lower (~0.2 eV) reaction barrier for TS1 relative to PBE but a slightly higher energy (~0.1 eV) for IM14 and TS15′. While the PBE results agree somewhat better with the SCAN+rvv10 results, we nevertheless investigated the effect of D3 correction on the microkinetic model by correcting the rate constants based on PBE with single point PBE-D3 energies. We note that the PBE-D3 energies and geometries of PBE-D3 and PBE optimized structures shown in Table S6 and Figure S9 differ by less than 0.003 eV. Figure S12 illustrates the PBE-D3 computed free energy profile that corresponds to Figure 4, and Table S7 summarizes the ZPE corrected PBE-D3 computed reaction energies and forward activation barriers. Next, Tables S8 and S9 illustrate the rate and equilibrium constants for all elementary reactions and the surface coverages of the microkinetic model at three different temperatures (748 K, 798 K and 823 K), respectively. In agreement to our previous PBE results, the PBE-D3 corrected microkinetic model (see Table S10) suggests that Path II is the dominant mechanism and the first C-H cleavage in propane is rate controlling. Also, the apparent activation barrier and the reaction orders remain essentially unchanged. Only the overall predicted activity of the $N_2O/NO_x$-type active site is predicted to be about two orders of magnitude higher in the PBE-D3 corrected model relative to the PBE model. Thus, it is our expectation that the trends, rates, and conclusions reported in this paper for the ODHP on a $N_2O/NO_x$-type active site will not be overtly affected by the DFT functional.

## 4. CONCLUSIONS

In summation, combining DFT with microkinetic modeling techniques, we systematically investigated the ODHP reaction on oxygen passivated boron nitride nanoribbons (BNNRs) to identify a likely active site, as well as the reaction mechanism for the ODHP under experimental reaction conditions. BNNRs with three different edges such as (1) armchair edge (armBNNR), (2) zigzag edge (zzBNNR), and (3) modified zigzag edge (mzzBNNR) were considered. mzzBNNR is much less stable than armchair and zigzag BNNR in the bare form with the stability order: armBNNR > zzBNNR > mzzBNNR. However, a constrained thermodynamic analysis suggests that the mzzBNNR is the most stable structure in the presence of adsorbed oxygen and the stability order reverses to: O@mzzBNNR > O@zzBNNR > O@armBNNR. Thus, the least stable bare BN edge can eventually become the most stable edge structure after oxygen adsorption under experimental reaction conditions. Further analysis revealed that the B-edge of mzzBNNR prefers to be fully passivated with O atoms forming six membered rings, while the N-edge prefers to have only one adsorbed O atom per five-membered ring under the experimental reaction conditions considered here. Calculations predicted that the O passivated B-edge of mzzBNNR is inactive for propane activation, whereas the O passivated five-membered N-edge of mzzBNNR, with a $N_2O/NO_x$-type active site, can selectively catalyze the ODHP reaction.

To study the mechanism of the ODHP reaction over this $N_2O/NO_x$-type active site, we focused on a redox pathway in which $C_3H_8$ molecules react with the catalyst forming $C_3H_6$ and $H_2O$ molecules and leaving oxygen "vacancies" on the BNNR edge. These oxygen vacancies can be replenished by dissociative adsorption of $O_2$. Since our thermodynamic analysis predicted similar energies for the structures, BNNR12O, BNNR13O, and BNNR14O, three catalytic cycles were examined starting with each of these structures. Our microkinetic reactor analysis for the overall reaction network predicted a high TOF on the order of $10^{-2}$ $s^{-1}$ in the temperature range of

748 to 823 K for a catalytic reaction cycle between BNNR13O and BNNR11O, implying high activity of the $N_2O/NO_x$-type active site for ODHP. The reaction cycle between BNNR14O and BNNR12O was found to be inhibited by a high activation barrier required for the $O_2$ dissociation process on BNNR12O. In the case of a catalytic cycle between BNNR12O and BNNR10O, the energy required to create a second oxygen vacancy seems to be the limiting factor for its activity. A degree of rate control analysis suggested that the overall rate is controlled by the initial activation of propane which agrees well with experimental observations. However, the calculated apparent activation barrier and reaction orders were found to be somewhat different from the experimental reports which could be explained by the experiments measuring both the effect of temperature and species partial pressure on (i) the catalysis of the active site and (ii) the creation of the active site which is likely reaction condition dependent. Alternatively, gas phase reactions occurring in parallel to the surface catalyzed reactions might explain the reason for this discrepancy. In fact, calculations predicted that the rate limiting propane activation step can also generate a gas phase $C_3H_7^{\bullet}$ radical on the $N_2O/NO_x$-type active site on the BNNR edge under the reaction conditions considered here, which in turn can trigger a gas phase ODHP reaction as experimentally speculated. Importantly and in agreement with experimental observations, the $N_2O/NO_x$-type active site on the BNNR edge is selective for propene production, having a 0.2 eV higher barrier for propene activation relative to propane activation. Overall, the results imply that the proposed $N_2O/NO_x$-type active site on the BNNR edge is highly active and selective for the ODH of propane suggesting that nitrogen is possibly an essential element for this reaction. These results do not contradict the experimental reports hypothesizing that boron is the essential element, rather they show the importance of both N and B and a $N_2O/NO_x$-type active site on BNNR for the ODHP. Thus, we would like to encourage experimental groups to study the ODH of propane over the said

different boron-containing materials in the absence and presence of a molecular $N_2$ environment to test our hypothesis. In addition, we would like to encourage experimental groups to use microwave (MW) irradiation to heat the solid BN catalyst selectively during reaction while suppressing possible gas phase reactions (due to the lower gas phase temperature). In this way, it should become possible to clearly determine the specific role and function of the solid catalyst versus gas-phase reactions.

**Supporting Information**

Comparison of Gibbs free energy variation with O adsorption that start from B-edge and N-edge (Figure S1), different possible configurations and relative free energies after first C-H cleavage of $C_3H_8$ on the catalyst (Figure S2 & Table S1), energy profiles of overall ODHP reaction (Figure S3), possible H atom rearrangement pathways (Figure S4 & S6), TSs involved along the most crucial $13O \rightarrow 11O \rightarrow 13O$ reaction cycle of the overall reaction network (Figure S5), IMs and TS of $N_2$ desorption pathway (Figure S7), effect of partial pressure of reactant gases on the reaction rate (Figure S8), comparison of results obtained using PBE, PBE-D3, and SCAN+rvv10 functionals (Figure S9 & Table S6), Gibbs free energy ($\Delta G_{ads}$) of B loss (FigureS10), calculated Bader charges (Figure S11), free energy profiles with PBE-D3 (Figure S12), Arrhenius plot with PBE-D3 (Figure S13), effect of partial pressure of reactant gases on the reaction rate with PBE-D3 (Figure S14), relative (free) energies of propene activation barriers, $C_3H_7^\bullet$ radical formation, NO desorption, $N_2O$ desorption, and $N_2$ desorption pathway, respectively (Table S2), reaction energies and activation barriers for all the elementary steps involved in the microkinetic model (Table S3), forward rate constants and equilibrium constants calculated at different temperatures (Table S4), surface coverages of various intermediates calculated at different temperatures (Table

S5), reaction energies and activation barriers for all the elementary steps involved in the microkinetic model with PBE-D3 (Table S7), forward rate constants and equilibrium constants calculated at different temperatures with PBE-D3 (Table S8), surface coverages of various intermediates calculated at different temperatures with PBE-D3 (Table S9), results from microkinetic model with PBE-D3 (Table S10).

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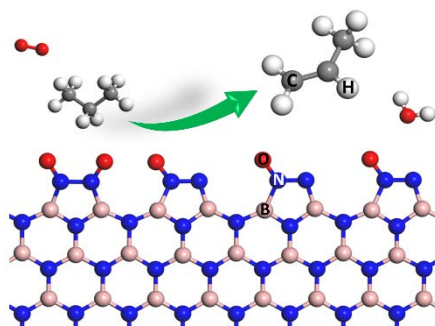
# Supporting Information of

# Oxidative Dehydrogenation of Propane on the Oxygen Adsorbed Edges of Boron Nitride Nanoribbons

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**(a)**



**(b)**
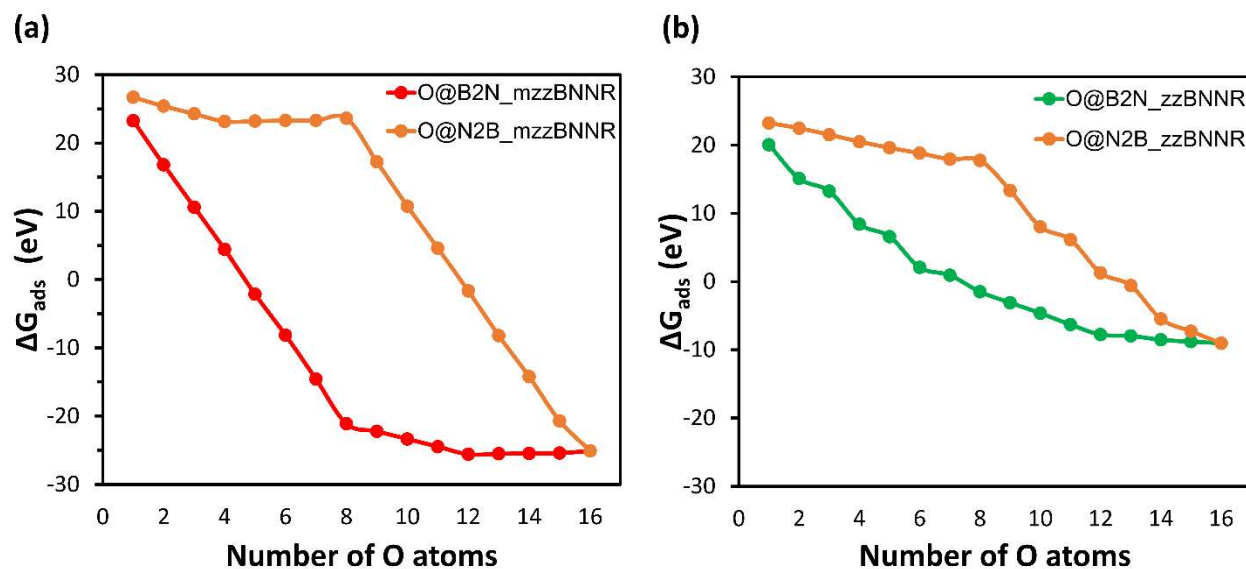


**Figure S1:** Gibbs free energy ($\Delta G_{ads}$) variation with O adsorption starting from B-edge (O@B2N) and N-edge (O@N2B) of (a) mzzBNNR and (b) zzBNNR. Color codes are shown in the corresponding inset and consistent with Figure 2 of the main manuscript. All energies are with reference to the sum of the energies of the optimized unit cell of bare armBNNR and molecular oxygen (T = 800 K and $P_{O_2}$ = 0.15 atm).
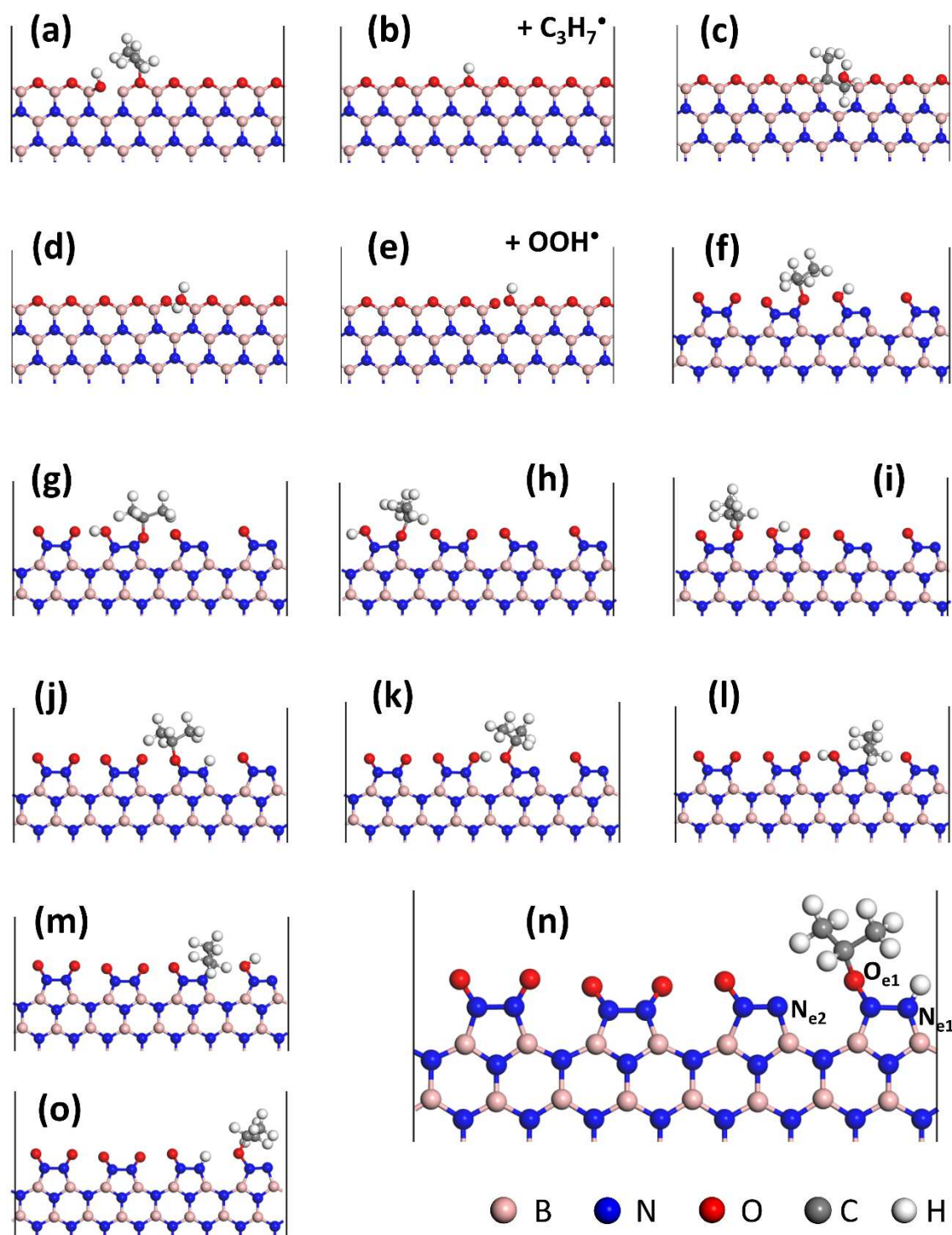
**Figure S2:** Relaxed structures of different possible configurations after first C-H cleavage of $C_3H_8$ on different sites of BNNR14O edges: (a) P1 (b) P2 (c) P3 (d) P4 (e) P5 (f) P6 (g) P7 (h) P8 (i) P9 (j) P10 (k) P11 (l) P12 (m) P13 (n) P14 (o) P15. (a)-(e) are structures on the B-edge, while all others are on the N-edge. The edge N and O atoms involved in H abstraction from $C_3H_8$ are denoted in the inset of the most stable intermediate P14 (n). Color code of the atoms is shown in the inset.
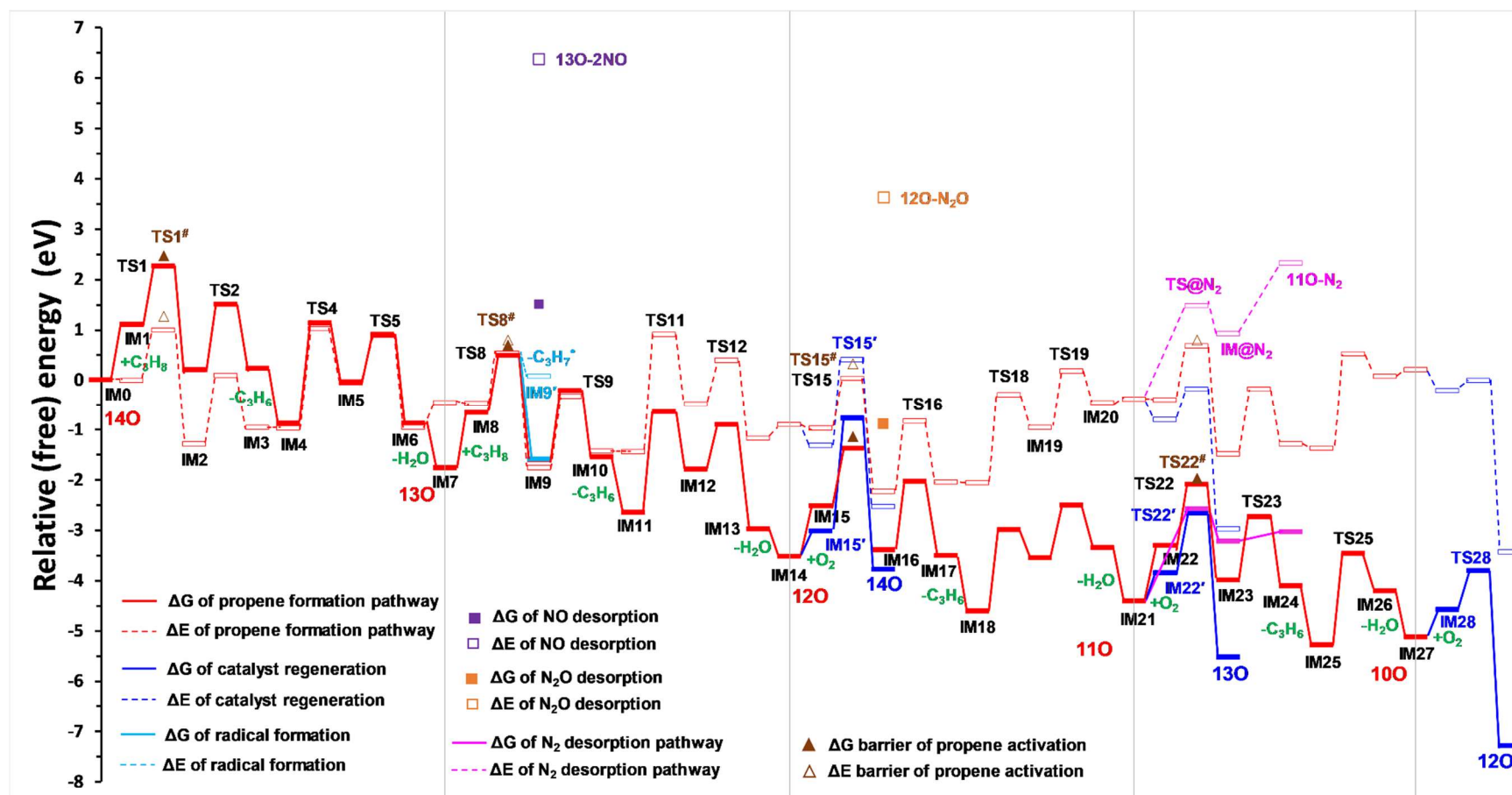
**Figure S3:** Free energy and zero-point energy (ZPE) corrected energy profiles for ODHP reaction on the O@mzzBNNR catalyst, denoted by solid and dashed lines, respectively. All free energies are calculated with reference to the sum of the energies of BNNR14O and the reactant gas molecules. Color code of the pathways is shown in the inset. T = 800 K, $P_{C_3H_8}$ = 0.3 atm, $P_{O_2}$ = 0.15 atm, $P_{C_3H_6}$ = 0.3 atm, $P_{C_3H_7^\bullet}$ = 0.3 atm, $P_{N_2}$ = 0.55 atm, $P_{N_2O}$ = 0.001 atm, and $P_{NO}$ = 0.001 atm. Relative free energies and ZPE corrected energies of the propene activation barriers (TS1#, TS8#, TS15# and TS22#), $C_3H_7^\bullet$ radical formation (IM9′), NO desorption (13O-2NO), N$_2$O desorption (12O-N$_2$O), and N$_2$ desorption pathway (TS@N$_2$, IM@N$_2$ and 11O-N$_2$) processes, of this figure and Figure 4 of the main manuscript, which are not included and corresponding processes, for comparison, which are included in the microkinetic model are tabulated in Table S2 of Supporting Information.
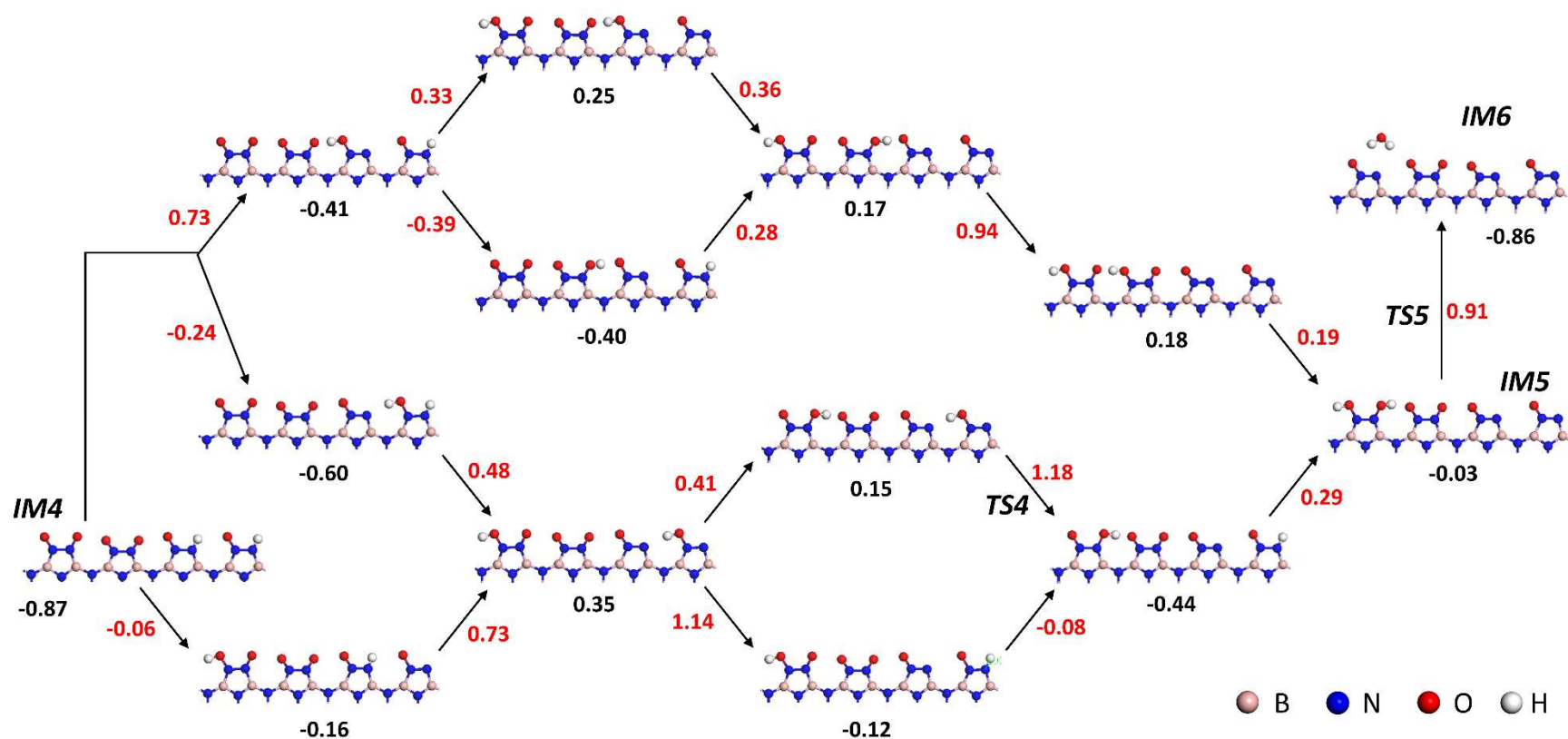
**Figure S4:** Possible H atom rearrangement pathways, from IM4 to IM6 of Figure 4, along with the optimized structures of the intermediates, and corresponding relative free energies (T = 800 K, $P_{C_3H_8}$ = 0.3 atm, and $P_{O_2}$ = 0.15 atm) of the intermediates (black) and TSs (red), respectively. All free energies are calculated with reference to the sum of the energies of BNNR14O and the reactant gas molecules, $C_3H_8$ and $O_2$. Color code of the atoms is shown in the inset.
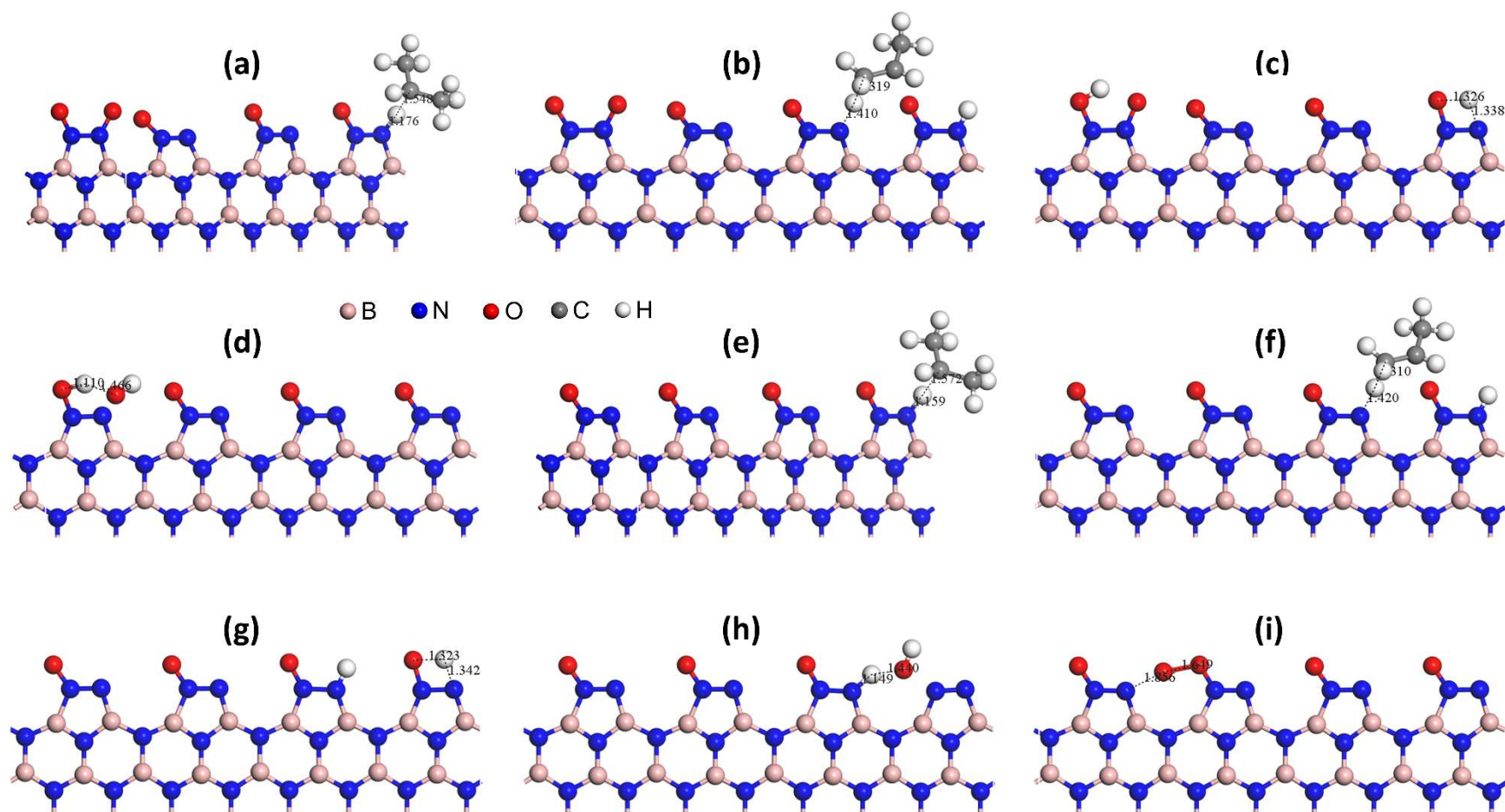
**Figure S5:** Relaxed structures of TSs involved along the most crucial 13O→11O→13O reaction cycle (Figure 5 of main manuscript): (a) TS8 (b) TS9 (c) TS11 (d) TS12 (e) TS15 (f) TS16 (g) TS18 (h) TS19 (i) TS22′. Color code of the atoms is shown in the inset.
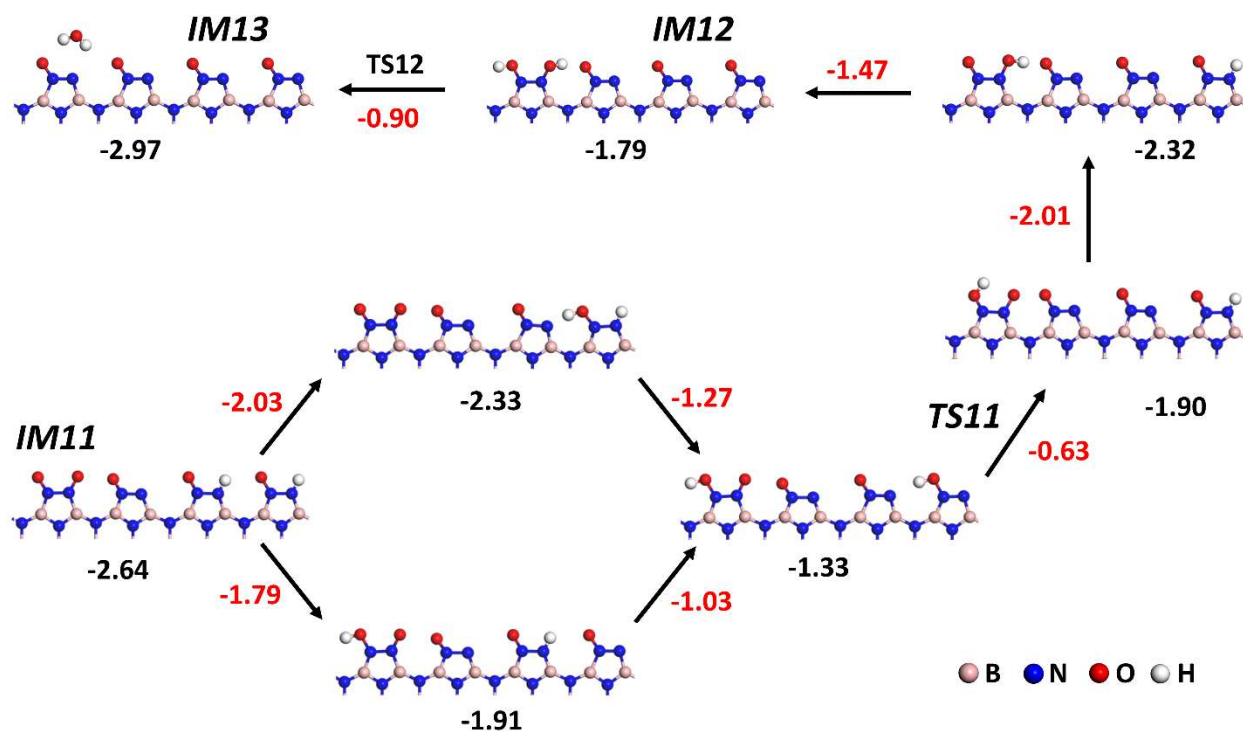
**Figure S6:** Possible H atom rearrangement pathways, from IM11 to IM13 of Figure 5, along with the optimized structures of intermediates and corresponding relative free energies (T = 800 K, $P_{C_3H_8}$ = 0.3 atm, and $P_{O_2}$ = 0.15 atm) of the intermediates (black) and TSs (red), respectively. All free energies are calculated with reference to the sum of the energies of BNNR14O and the reactant gas molecules, $C_3H_8$ and $O_2$. Color code of the atoms is shown in the inset.
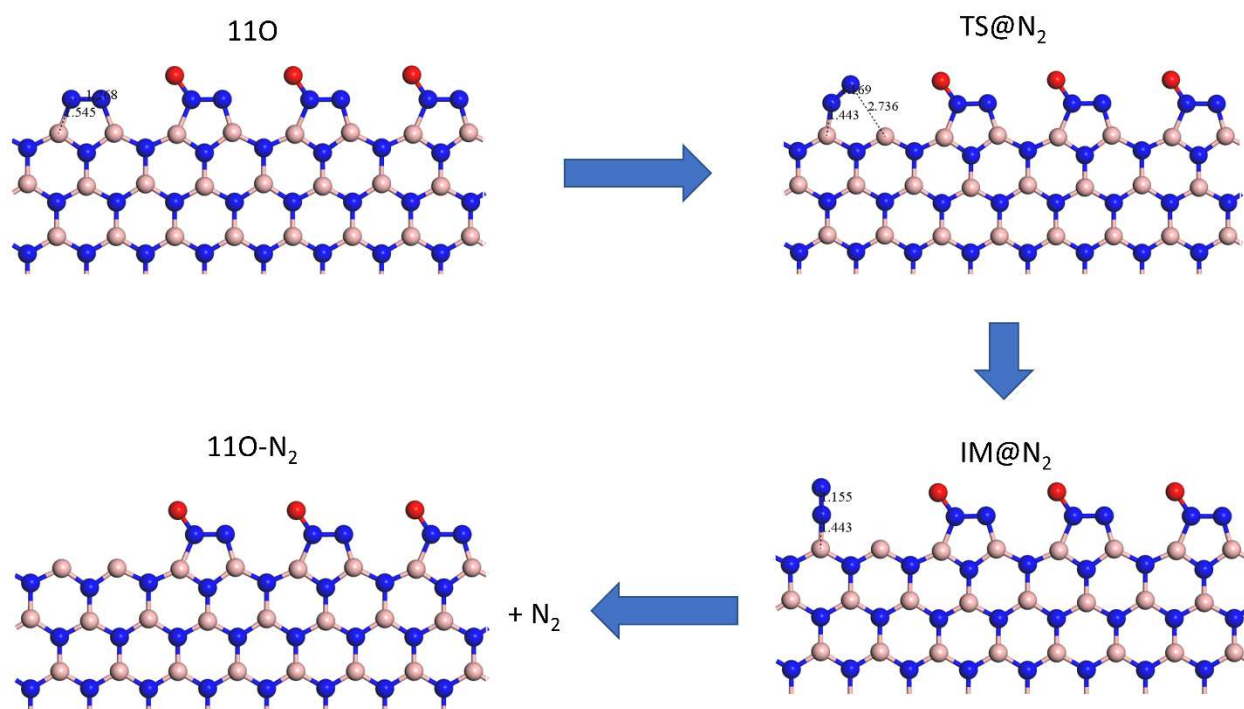
**Figure S7:** Relaxed structures of intermediates and transition state structures involved in the $N_2$ desorption pathway from 11O.
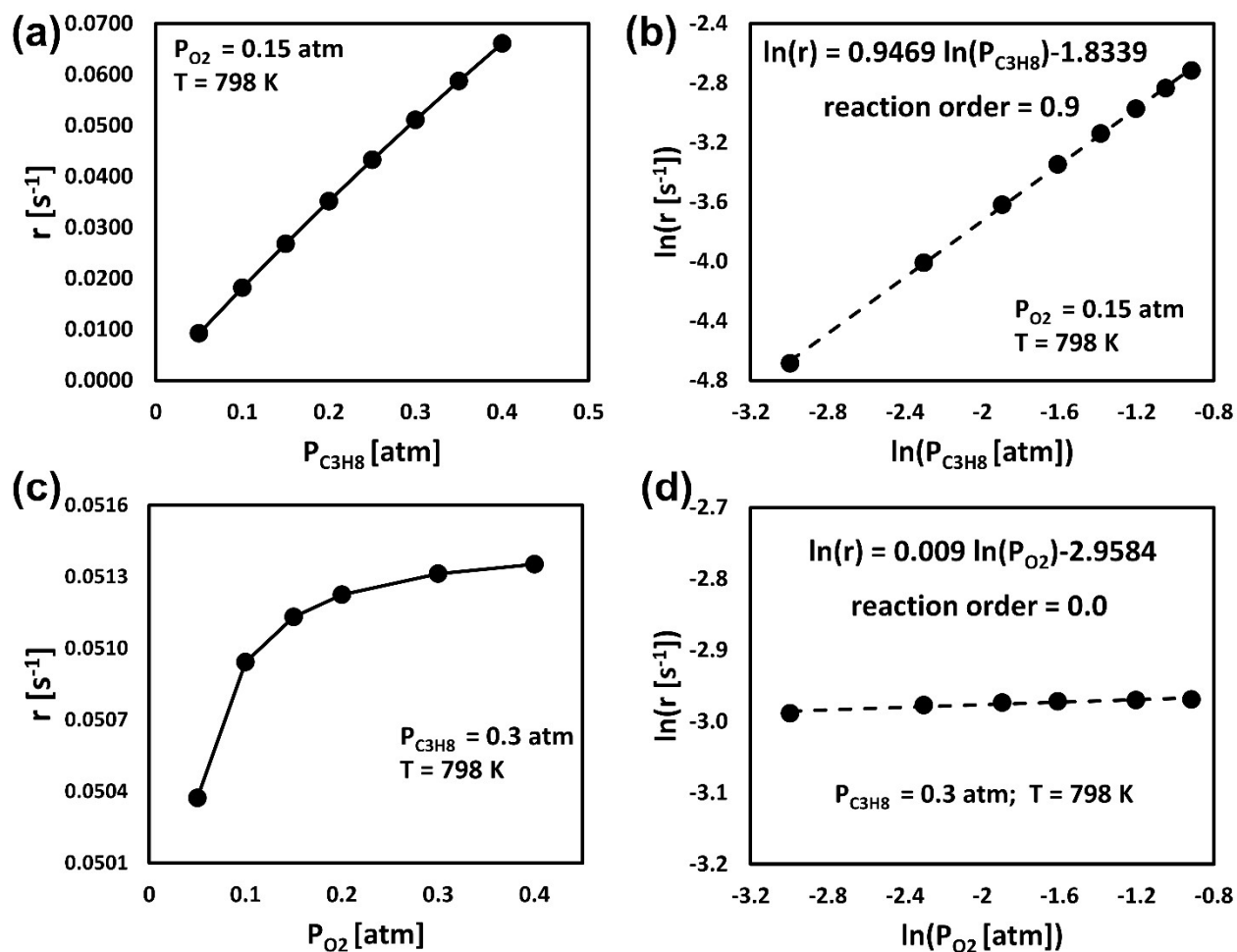
**Figure S8:** Effect of partial pressure of (a and b) $C_3H_8$ and (c and d) $O_2$ on the reaction rate (r [s$^{-1}$]) of the overall reaction, respectively, at T = 798 K.
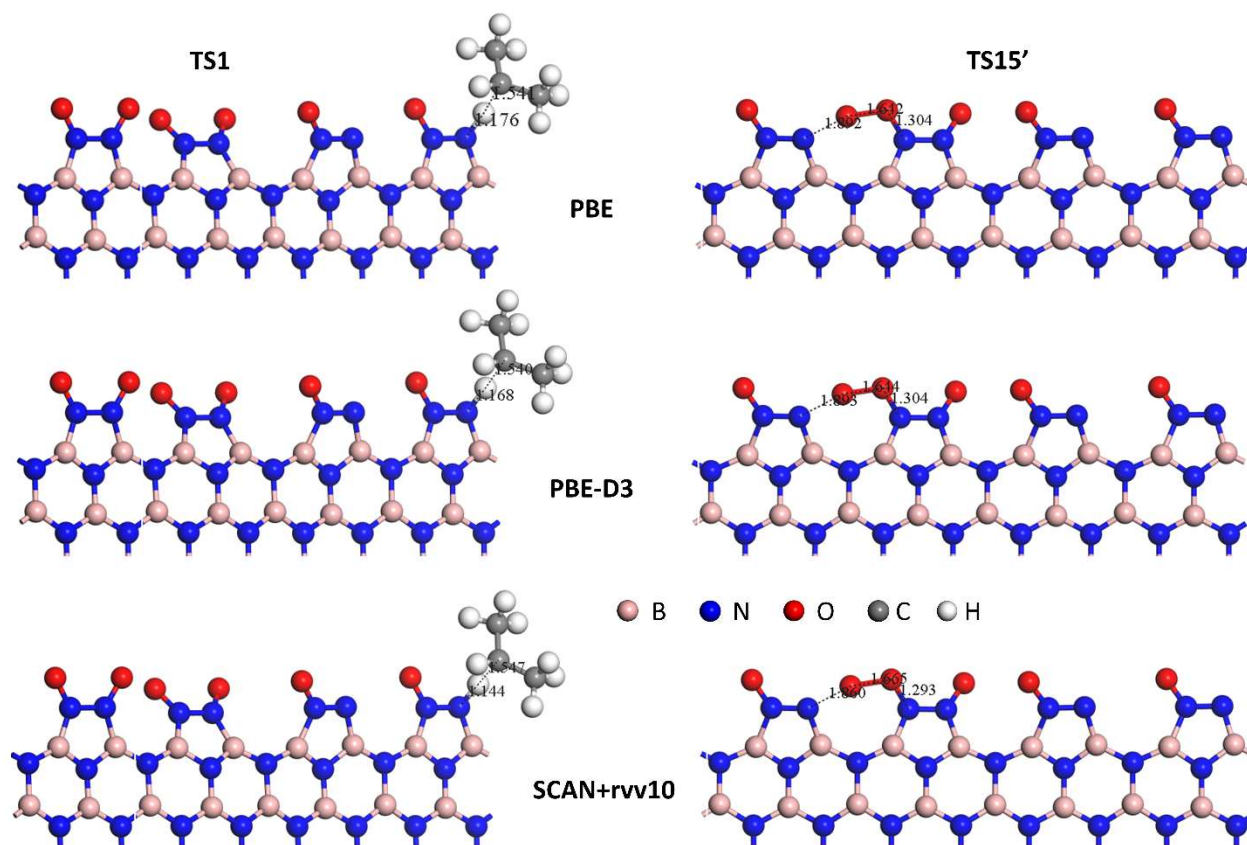
**Figure S9:** Transition state structures involved in the propane activation on BNNR14O (TS1) and O$_2$ dissociation over BNNR12O (TS15′) calculated using PBE (top), PBE-D3 (middle), and SCAN+rvv10 (bottom) functionals.
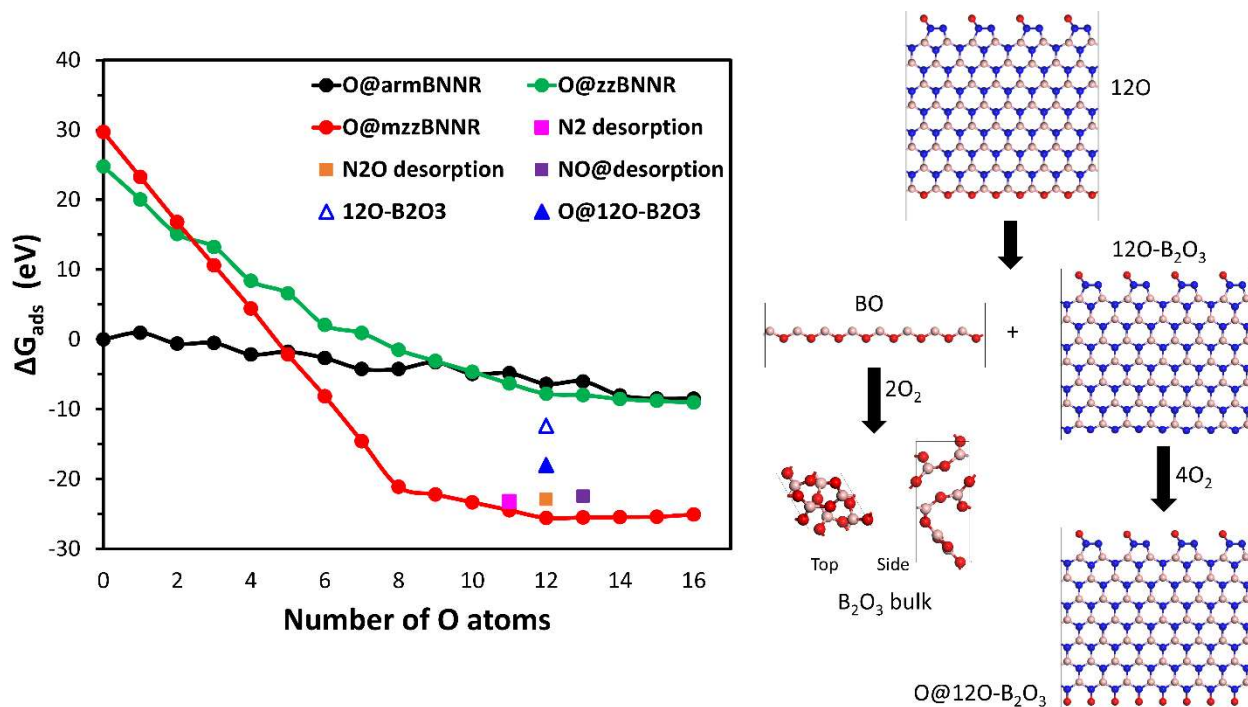
**Figure S10:** Gibbs free energy ($\Delta G_{ads}$) of B loss from BNNR12O (shown in blue triangles) compared with the free energy of O passivation on the edges of the three BNNRs and $N_2$, NO and $N_2O$ desorption from the considered catalysts. Color codes are shown in the corresponding inset. All free energies are calculated with reference to the energy of the optimized unit cell of bare armchair BNNR at T = 800 K and $P_{O_2}$ = 0.15 atm. $P_{N_2}$ = 0.55 atm, $P_{N_2O}$ = 0.001 atm, and $P_{NO}$ = 0.001 atm. The optimized structures of the 1D BO, the nanoribbon after BO removal (12O-$B_2O_3$), the fully oxygen passivated nanoribbon after BO removal (O@12O-$B_2O_3$), and the unit-cell of bulk $B_2O_3$ are also shown on the right. One unit-cell of bulk $B_2O_3$ is composed of 6 B and 9 O atoms. Thus, to get the free energy for one-unit $B_2O_3$ we divided the energy of the bulk $B_2O_3$ unit-cell by 3. On the other hand, the one-dimensional BO precursor has 8 B and 8 O atoms. In the free energy calculation, we consider the energy of the precursor as $8BO = 4B_2O_3 - 2O_2$.
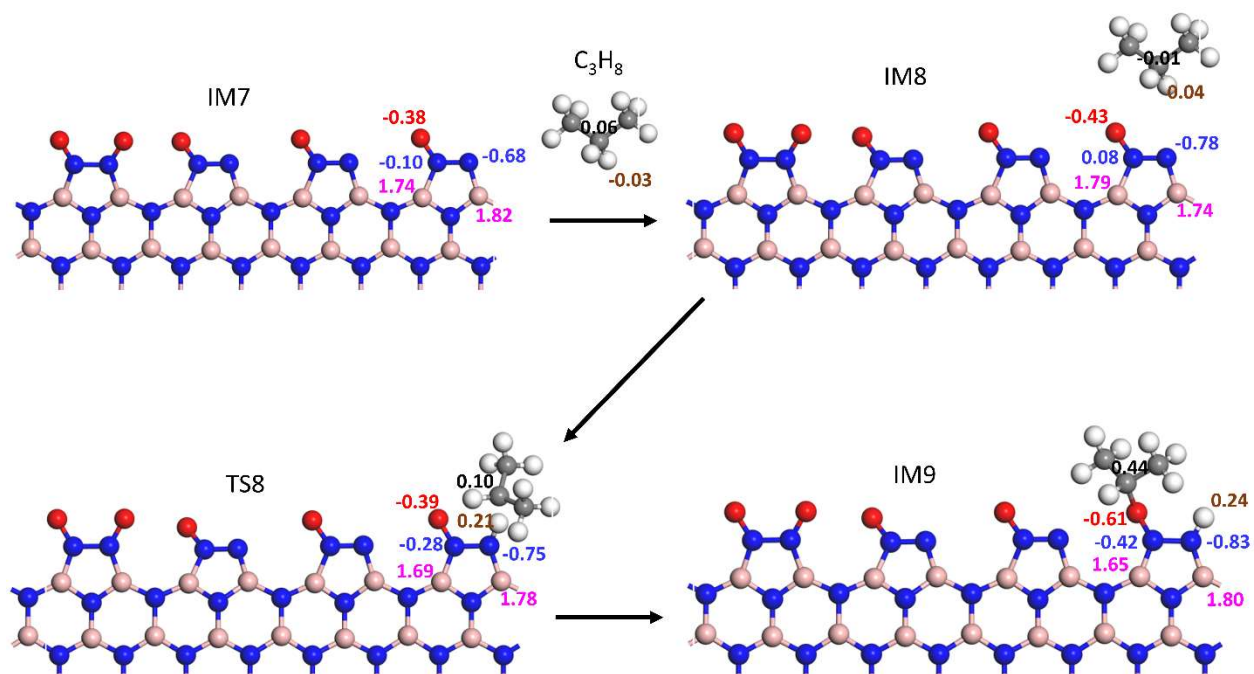
**Figure S11:** Calculated Bader charge of the edge atoms of the five-membered ring and the reactant propane for IM7, IM8, TS8, and IM9 of the proposed reaction mechanism for the ODHP.
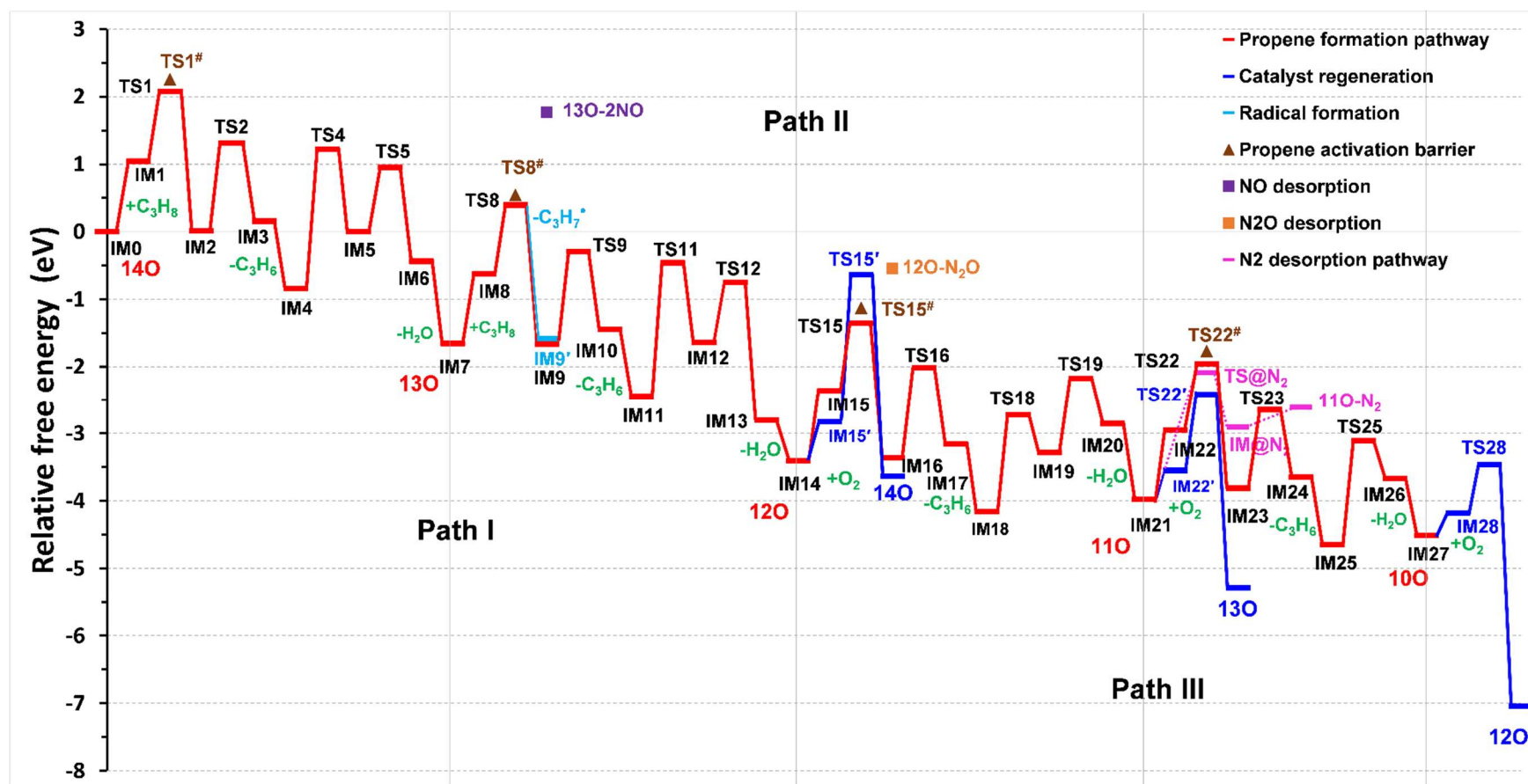
**Figure S12:** Free energy profiles for three different (coupled) catalytic cycles (Path I: 14O to 12O; Path II: 13O to 11O; and Path III: 12O to 10O) of the ODHP reaction on the O@mzzBNNR catalysts form single point PBE-D3 calculations. The color code of the different parts of the pathways are shown in the inset. All free energies are calculated with reference to the sum of the energies of BNNR14O and the reactant gas molecules, at T = 800 K, $P_{C_3H_8}$ = 0.3 atm, $P_{O_2}$ = 0.15 atm, $P_{C_3H_6}$ = 0.3 atm, $P_{C_3H_7^\bullet}$ = 0.3 atm, $P_{N_2}$ = 0.55 atm, $P_{N_2O}$ = 0.001 atm, and $P_{NO}$ = 0.001 atm.
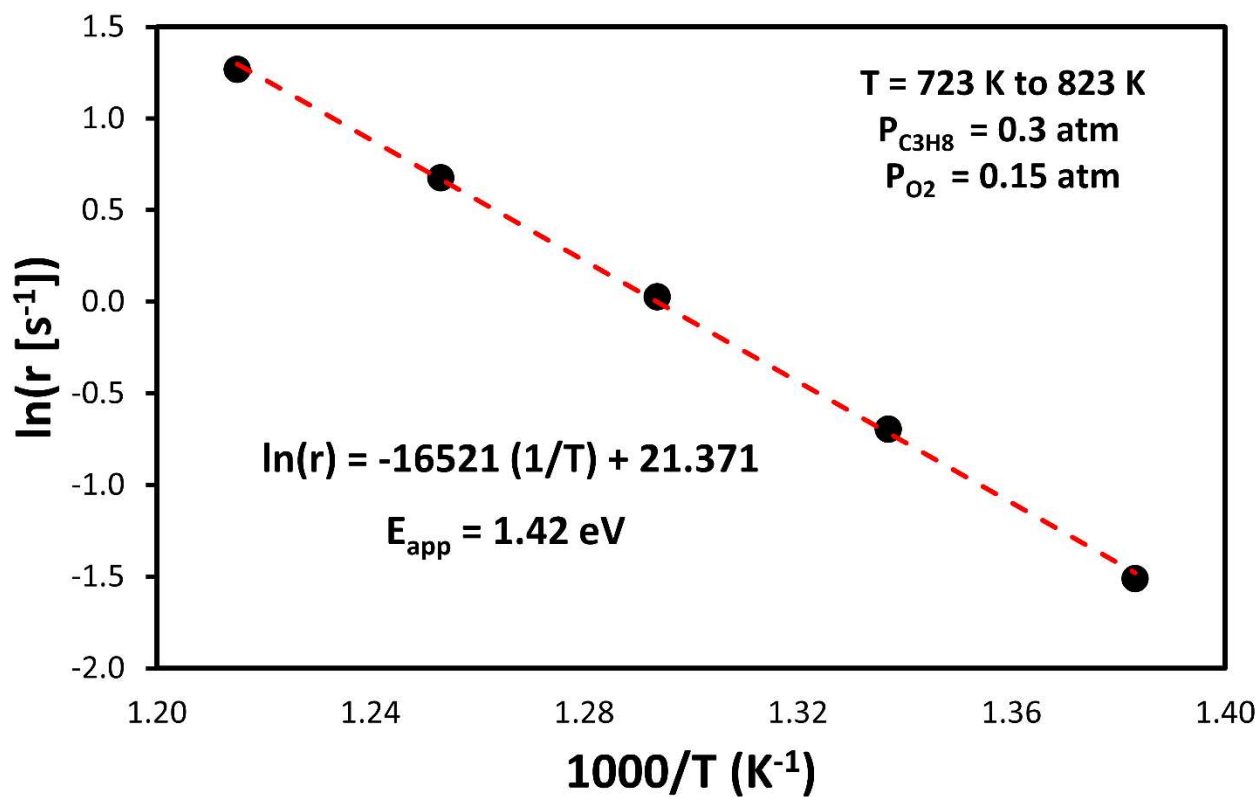
**Figure S13:** Arrhenius plot for the overall reaction based on energies computed using the PBE-D3 functional, revealing an apparent activation energy of 1.34 eV in a temperature range of 723 to 823 K, and $P_{C_3H_8} = 0.3$ atm, $P_{O_2} = 0.15$ atm.
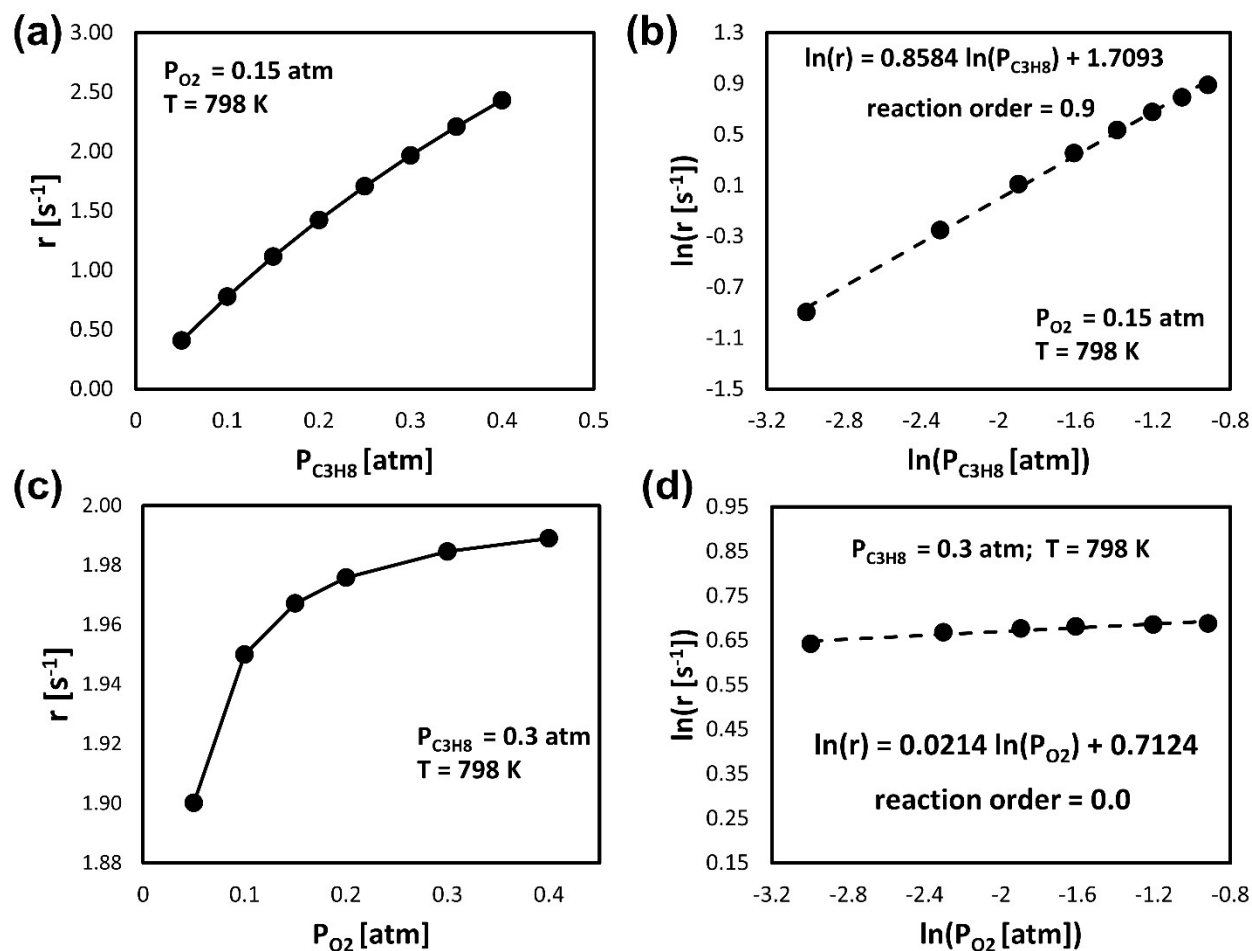
**Figure S14:** Effect of partial pressure of (a and b) $C_3H_8$ and (c and d) $O_2$ on the reaction rate (r [s⁻¹]) of the overall reaction, respectively, at T = 798 K. Data are based on a microkinetic model based on PBE-D3 single point calculations.

**Table S1:** Calculated relative free energies and ZPE corrected energies of different possible configurations (P1 to P15) after first C-H cleavage of $C_3H_8$ on different sites of the BNNR14O edge. All energies are referenced to the sum of the energies of BNNR14O and a gas phase $C_3H_8$ molecule. Free energies are computed at T= 800 K, $P_{C_3H_8}$ = 0.3 atm, $P_{H_2O}$ = 0.3 atm, $P_{O_2}$ = 0.15 atm, and $P_{O_2H\bullet}$ = 0.15 atm.

| Possible intermediate structures | P1 | P2 | P3 | P4 | P5 | P6 |
|---|---|---|---|---|---|---|
| **ΔG (eV)** | 7.21 | 4.18 | 2.58 | 1.17 | 3.08 | 1.50 |
| **ΔE (eV)** | 5.73 | 4.63 | 1.19 | -0.17 | 1.96 | 0.06 |
| **Possible intermediate structures** | P7 | P8 | P9 | P10 | P11 | P12 |
| **ΔG (eV)** | 0.89 | 1.10 | 1.44 | 0.24 | 1.37 | 0.26 |
| **ΔE (eV)** | -0.61 | -0.40 | -0.09 | -1.24 | -0.14 | -1.23 |
| **Possible intermediate structures** | P13 | P14 | P15 | | | |
| **ΔG (eV)** | 1.05 | 0.20 | 0.82 | | | |
| **ΔE (eV)** | -0.51 | -1.28 | -0.61 | | | |

**Table S2:** Relative free energies ($\Delta$**G**) and ZPE corrected energies ($\Delta E_{ZPE}$) of the propene activation barriers (TS1#, TS8#, TS15# and TS22#), $C_3H_7^\bullet$ radical formation (IM9′), NO desorption (13O-2NO), $N_2O$ desorption (12O-$N_2O$), and $N_2$ desorption pathway (TS@$N_2$, IM@$N_2$ and 11O-$N_2$) as shown in Figure 4 of the main manuscript and Figure S3 of Supporting Information. These pathways are not included in the microkinetic model considered in the present work. For comparison, the $\Delta$G and $\Delta E_{ZPE}$ of corresponding important states, which are included in the microkinetic model, are also tabulated. All free energies are calculated with reference to the sum of the energies of BNNR14O and the reactant gas molecules at T = 800 K, $P_{C_3H_8}$ = 0.3 atm, $P_{O_2}$ = 0.15 atm, $P_{C_3H_6}$ = 0.3 atm, $P_{C_3H_7^\bullet}$ = 0.3 atm, $P_{N_2}$ = 0.55 atm, $P_{N_2O}$ = 0.001 atm, and $P_{NO}$ = 0.001 atm.

| Structures | $\Delta$**G (eV)** | $\Delta E_{ZPE}$ **(eV)** |
|---|---|---|
| BNNR14O (IM0) | 0.00 | 0.00 |
| TS1 | 2.27 | 0.99 |
| TS1# | 2.47 | 1.26 |
| BNNR13O (IM7) | -1.75 | -0.45 |
| TS8 | 0.49 | 0.54 |
| TS8# | 0.69 | 0.79 |
| IM9 | -1.60 | -1.76 |
| IM9′ | -1.58 | 0.07 |
| 13O-2NO | 1.49 | 6.37 |
| BNNR12O (IM14) | -3.52 | -0.90 |
| TS15 | -1.37 | 0.03 |
| TS8# | -1.14 | 0.32 |
| 12O-$N_2O$ | -0.89 | 3.61 |
| BNNR11O (IM21) | -4.40 | -0.39 |
| TS22 | -2.08 | 0.68 |
| TS22# | -1.98 | 0.79 |
| TS22′ | -2.66 | -0.18 |
| TS@$N_2$ | -2.57 | 1.48 |
| IM@$N_2$ | -3.22 | 0.92 |
| 11O-$N_2$ | -3.03 | 2.32 |

**Table S3:** ZPE corrected reaction energies ($\Delta E_{ZPE}^{rxn}$), forward activation barriers ($\Delta E_{ZPE}^{act}$), and calculated imaginary vibrational frequencies for the corresponding transition state of the elementary steps considered in the overall reaction network of the ODHP reaction.

| | Reaction | $\Delta E_{ZPE}^{rxn}$ (eV) | $\Delta E_{ZPE}^{act}$ (eV) | Frequency (i) (cm$^{-1}$) |
|---|---|---|---|---|
| (R1) | BNNR14O (IM0) + $C_3H_{8\,(g)}$ → BNNR14O-$C_3H_8$ (IM1) | -0.01 | - | |
| (R2) | BNNR14O-$C_3H_8$ (IM1) → BNNR14O-$C_3H_7$-H (IM2) | -1.27 | 1.00 | 987 |
| (R3) | BNNR14O-$C_3H_7$-H (IM2) → BNNR14O-2H-$C_3H_6$ (IM3) | 0.33 | 1.37 | 1184 |
| (R4) | BNNR14O-2H-$C_3H_6$ (IM3) → BNNR14O-2H (IM4) + $C_3H_{6\,(g)}$ | -0.01 | - | |
| (R5) | BNNR14O-2H (IM4) → BNNR14O-2Hr (IM5) | 0.92 | 1.99 | 1736 |
| (R6) | BNNR14O-2Hr (IM5) → BNNR13O-$H_2O$ (IM6) | -0.90 | 0.95 | 722 |
| (R7) | BNNR13O-$H_2O$ (IM6) → BNNR13O (IM7) + $H_2O_{(g)}$ | 0.50 | - | |
| (R8) | BNNR13O (IM7) + $C_3H_{8\,(g)}$ → BNNR13O-$C_3H_8$ (IM8) | -0.02 | - | |
| (R9) | BNNR13O-$C_3H_8$ (IM8) → BNNR13O-$C_3H_7$-H (IM9) | -1.29 | 1.00 | 992 |
| (R10) | BNNR13O-$C_3H_7$-H (IM9) → BNNR13O-2H-$C_3H_6$ (IM10) | 0.34 | 1.44 | 1255 |
| (R11) | BNNR13O-2H-$C_3H_6$ (IM10) → BNNR13O-2H (IM11) + $C_3H_{6\,(g)}$ | -0.02 | - | |
| (R12) | BNNR13O-2H (IM11) → BNNR13O-2Hr (IM12) | 0.95 | 2.01 | 1736 |
| (R13) | BNNR13O-2Hr (IM12) → BNNR12O-$H_2O$ (IM13) | -0.68 | 0.89 | 674 |
| (R14) | BNNR12O-$H_2O$ (IM13) → BNNR12O (IM14) + $H_2O_{(g)}$ | 0.20 | - | |
| (R15) | BNNR12O (IM14) + $C_3H_{8\,(g)}$ → BNNR12O-$C_3H_8$ (IM15) | -0.01 | - | |
| (R16) | BNNR12O-$C_3H_8$ (IM15) → BNNR12O-$C_3H_7$-H (IM16) | -1.25 | 1.00 | 857 |
| (R17) | BNNR12O-$C_3H_7$-H (IM16) → BNNR12O-2H-$C_3H_6$ (IM17) | 0.19 | 1.41 | 1399 |
| (R18) | BNNR12O-2H-$C_3H_6$ (IM17) → BNNR12O-2H (IM18) + $C_3H_{6\,(g)}$ | -0.02 | - | |
| (R19) | BNNR12O-2H (IM18) → BNNR12O-2Hr (IM19) | 1.11 | 1.88 | 1721 |
| (R20) | BNNR12O-2Hr (IM19) → BNNR11O-$H_2O$ (IM20) | 0.50 | 1.13 | 2105 |
| (R21) | BNNR11O-$H_2O$ (IM20) → BNNR11O (IM21) + $H_2O_{(g)}$ | 0.06 | - | |
| (R22) | BNNR11O (IM21) + $O_{2\,(g)}$ → BNNR11O-$O_2$ (IM22′) | -0.41 | - | |
| (R23) | BNNR11O-$O_2$ (IM22′) → BNNR13O (IM7) | -2.18 | 0.62 | 526 |
| (R24) | BNNR11O (IM21) + $C_3H_{8\,(g)}$ → BNNR11O-$C_3H_8$ (IM22) | -0.01 | - | |
| (R25) | BNNR11O-$C_3H_8$ (IM22) → BNNR11O-$C_3H_7$-H (IM23) | -1.08 | 1.07 | 844 |
| (R26) | BNNR11O-$C_3H_7$-H (IM23) → BNNR11O-2H-$C_3H_6$ (IM24) | 0.20 | 1.30 | 1338 |
| (R27) | BNNR11O-2H-$C_3H_6$ (IM24) → BNNR11O-2H (IM25) + $C_3H_{6\,(g)}$ | -0.09 | - | |
| (R28) | BNNR11O-2H (IM25) → BNNR10O-$H_2O$ (IM26) | 1.44 | 1.90 | 890 |
| (R29) | BNNR10O-$H_2O$ (IM26) → BNNR10O (IM27) + $H_2O_{(g)}$ | 0.13 | - | |
| (R30) | BNNR10O (IM27) + $O_{2\,(g)}$ → BNNR10O-$O_2$ (IM28) | -0.41 | - | |

| | | | |
|---|---|---|---|
| (R31)   BNNR10O-O$_2$ (IM28) → BNNR12O (IM14) | -3.28 | 0.19 | 513 |
| (R32)   BNNR12O (IM14) + O$_{2\,(g)}$ → BNNR12O-O$_2$ (IM15′) | -0.44 | - | |
| (R33)   BNNR12O-O$_2$ (IM15′) → BNNR14O (IM0) | -1.11 | 1.82 | 470 |

**Table S4:** Forward rate constants ($k_{for}$) and equilibrium constants ($K$) calculated at different temperatures for the elementary steps considered in overall reaction network of the ODHP reaction ($P_{C_3H_8} = 0.3$ atm and $P_{O_2} = 0.15$ atm).

| Reaction | T= 748 K | | T = 798 K | | T = 823 K | |
|---|---|---|---|---|---|---|
| | $k_{for}$ (s$^{-1}$) | $K$ | $k_{for}$ (s$^{-1}$) | $K$ | $k_{for}$ (s$^{-1}$) | $K$ |
| R1 | $3.03\times10^9$ | $9.36\times10^{-8}$ | $2.94\times10^9$ | $1.04\times10^{-7}$ | $2.89\times10^9$ | $1.09\times10^{-7}$ |
| R2 | $2.94\times10^5$ | $1.99\times10^6$ | $8.17\times10^5$ | $5.52\times10^5$ | $1.30\times10^6$ | $3.08\times10^5$ |
| R3 | $2.13\times10^4$ | $4.20\times10^{-1}$ | $8.81\times10^4$ | $6.22\times10^{-1}$ | $1.68\times10^5$ | $7.44\times10^{-1}$ |
| R4 | $2.75\times10^{16}$ | $8.87\times10^6$ | $2.38\times10^{16}$ | $7.93\times10^6$ | $2.24\times10^{16}$ | $7.57\times10^6$ |
| R5 | $5.08\times10^{-1}$ | $2.28\times10^{-6}$ | $3.61$ | $5.55\times10^{-6}$ | $8.81$ | $8.31\times10^{-6}$ |
| R6 | $1.82\times10^6$ | $4.09\times10^5$ | $4.70\times10^6$ | $1.69\times10^5$ | $7.25\times10^6$ | $1.13\times10^5$ |
| R7 | $1.03\times10^{15}$ | $2.18\times10^5$ | $1.65\times10^{15}$ | $3.60\times10^5$ | $2.06\times10^{15}$ | $4.55\times10^5$ |
| R8 | $3.03\times10^9$ | $1.01\times10^{-7}$ | $2.94\times10^9$ | $1.13\times10^{-7}$ | $2.89\times10^9$ | $1.17\times10^{-7}$ |
| R9 | $3.74\times10^5$ | $3.68\times10^6$ | $1.04\times10^6$ | $1.00\times10^6$ | $1.66\times10^6$ | $5.54\times10^5$ |
| R10 | $5.84\times10^3$ | $2.75\times10^{-1}$ | $2.59\times10^4$ | $4.10\times10^{-1}$ | $5.10\times10^4$ | $4.93\times10^{-1}$ |
| R11 | $3.41\times10^{16}$ | $1.10\times10^7$ | $2.95\times10^{16}$ | $9.82\times10^6$ | $2.77\times10^{16}$ | $9.36\times10^6$ |
| R12 | $4.03\times10^{-1}$ | $5.60\times10^{-7}$ | $2.92$ | $1.40\times10^{-6}$ | $7.17$ | $2.13\times10^{-6}$ |
| R13 | $7.12\times10^7$ | $1.17\times10^8$ | $1.82\times10^8$ | $6.75\times10^7$ | $2.80\times10^8$ | $5.26\times10^7$ |
| R14 | $4.82\times10^{13}$ | $1.02\times10^4$ | $5.15\times10^{13}$ | $1.12\times10^4$ | $5.34\times10^{13}$ | $1.18\times10^4$ |
| R15 | $3.03\times10^9$ | $9.18\times10^{-8}$ | $2.94\times10^9$ | $1.03\times10^{-7}$ | $2.89\times10^9$ | $1.07\times10^{-7}$ |
| R16 | $3.80\times10^5$ | $1.24\times10^6$ | $1.06\times10^6$ | $3.52\times10^5$ | $1.69\times10^6$ | $1.98\times10^5$ |
| R17 | $1.09\times10^4$ | $3.86$ | $4.68\times10^4$ | $5.02$ | $9.10\times10^4$ | $5.66$ |
| R18 | $3.13\times10^{16}$ | $1.01\times10^7$ | $2.69\times10^{16}$ | $8.96\times10^6$ | $2.52\times10^{16}$ | $8.53\times10^6$ |
| R19 | $5.98$ | $6.43\times10^{-8}$ | $4.01\times10^1$ | $1.90\times10^{-7}$ | $9.52\times10^1$ | $3.11\times10^{-7}$ |
| R20 | $1.28\times10^6$ | $2.84\times10^{-2}$ | $4.07\times10^6$ | $4.94\times10^{-2}$ | $6.89\times10^6$ | $6.36\times10^{-2}$ |
| R21 | $2.00\times10^{16}$ | $4.22\times10^6$ | $1.96\times10^{16}$ | $4.26\times10^6$ | $1.95\times10^{16}$ | $4.32\times10^6$ |
| R22 | $1.78\times10^9$ | $4.37\times10^{-4}$ | $1.72\times10^9$ | $3.20\times10^{-4}$ | $1.69\times10^9$ | $2.77\times10^{-4}$ |
| R23 | $3.20\times10^5$ | $3.68\times10^{11}$ | $5.52\times10^5$ | $4.07\times10^{10}$ | $7.07\times10^5$ | $1.49\times10^{10}$ |
| R24 | $3.03\times10^9$ | $1.18\times10^{-7}$ | $2.94\times10^9$ | $1.32\times10^{-7}$ | $2.89\times10^9$ | $1.38\times10^{-7}$ |

| | | | | | | |
|------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| R25  | $9.59\times10^4$     | $6.42\times10^4$     | $2.84\times10^5$     | $2.14\times10^4$     | $4.67\times10^5$     | $1.29\times10^4$     |
| R26  | $4.30\times10^4$     | 3.77                 | $1.67\times10^5$     | 4.96                 | $3.11\times10^5$     | 5.62                 |
| R27  | $8.97\times10^{16}$  | $2.89\times10^7$     | $7.21\times10^{16}$  | $2.40\times10^7$     | $6.54\times10^{16}$  | $2.21\times10^7$     |
| R28  | 7.19                 | $3.24\times10^{-8}$  | $4.88\times10^1$     | $1.43\times10^{-7}$  | $1.17\times10^2$     | $2.81\times10^{-7}$  |
| R29  | $2.45\times10^{15}$  | $5.16\times10^5$     | $2.53\times10^{15}$  | $5.51\times10^5$     | $2.59\times10^{15}$  | $5.73\times10^5$     |
| R30  | $1.78\times10^9$     | $5.58\times10^{-4}$  | $1.72\times10^9$     | $4.10\times10^{-4}$  | $1.69\times10^9$     | $3.56\times10^{-4}$  |
| R31  | $2.05\times10^8$     | $1.56\times10^{19}$  | $2.31\times10^8$     | $5.77\times10^{17}$  | $2.44\times10^8$     | $1.29\times10^{17}$  |
| R32  | $1.78\times10^9$     | $8.16\times10^{-4}$  | $1.72\times10^9$     | $5.77\times10^{-4}$  | $1.69\times10^9$     | $4.92\times10^{-4}$  |
| R33  | $4.80\times10^{-3}$  | $4.77\times10^4$     | $2.73\times10^{-2}$  | $1.53\times10^4$     | $6.01\times10^{-2}$  | $9.13\times10^3$     |

**Table S5:** Surface coverage/probability density ($\theta$) of various intermediates calculated at different temperatures for overall pathway of the ODHP reaction ($P_{C3H8}$= 0.3, and $P_{O2}$= 0.15 atm).

| Intermediate | | Surface Coverage ($\theta$) | | |
|---|---|---|---|---|
| | | **748 K** | **798 K** | **823 K** |
| BNNR14O | (IM0) | $5.12 \times 10^{-5}$ | $7.35 \times 10^{-5}$ | $1.07 \times 10^{-4}$ |
| BNNR14O-C$_3$H$_8$ | (IM1) | $4.79 \times 10^{-12}$ | $7.66 \times 10^{-12}$ | $1.16 \times 10^{-11}$ |
| BNNR14O-C$_3$H$_7$-H | (IM2) | $6.77 \times 10^{-11}$ | $7.17 \times 10^{-11}$ | $9.05 \times 10^{-11}$ |
| BNNR14O-2H-C$_3$H$_6$ | (IM3) | $5.58 \times 10^{-13}$ | $4.09 \times 10^{-13}$ | $4.00 \times 10^{-13}$ |
| BNNR14O-2H | (IM4) | $4.95 \times 10^{-6}$ | $3.24 \times 10^{-6}$ | $3.03 \times 10^{-6}$ |
| BNNR14O-2Hr | (IM5) | $4.96 \times 10^{-12}$ | $8.48 \times 10^{-12}$ | $1.09 \times 10^{-11}$ |
| BNNR13O-H$_2$O | (IM6) | $1.71 \times 10^{-6}$ | $1.21 \times 10^{-6}$ | $9.91 \times 10^{-7}$ |
| BNNR13O | (IM7) | $3.72 \times 10^{-1}$ | $4.35 \times 10^{-1}$ | $4.51 \times 10^{-1}$ |
| BNNR13O-C$_3$H$_8$ | (IM8) | $3.77 \times 10^{-8}$ | $4.90 \times 10^{-8}$ | $5.29 \times 10^{-8}$ |
| BNNR13O-C$_3$H$_7$-H | (IM9) | $2.43 \times 10^{-6}$ | $1.98 \times 10^{-6}$ | $1.73 \times 10^{-6}$ |
| BNNR13O-2H-C$_3$H$_6$ | (IM10) | $3.22 \times 10^{-9}$ | $1.81 \times 10^{-9}$ | $1.33 \times 10^{-9}$ |
| BNNR13O-2H | (IM11) | $3.54 \times 10^{-2}$ | $1.77 \times 10^{-2}$ | $1.24 \times 10^{-2}$ |
| BNNR13O-2Hr | (IM12) | $1.99 \times 10^{-10}$ | $2.81 \times 10^{-10}$ | $3.16 \times 10^{-10}$ |
| BNNR12O-H$_2$O | (IM13) | $3.98 \times 10^{-5}$ | $4.21 \times 10^{-5}$ | $4.13 \times 10^{-5}$ |
| BNNR12O | (IM14) | $4.05 \times 10^{-1}$ | $4.72 \times 10^{-1}$ | $4.88 \times 10^{-1}$ |
| BNNR12O-C$_3$H$_8$ | (IM15) | $3.72 \times 10^{-8}$ | $4.84 \times 10^{-8}$ | $5.22 \times 10^{-8}$ |
| BNNR12O-C$_3$H$_7$-H | (IM16) | $1.30 \times 10^{-6}$ | $1.09 \times 10^{-6}$ | $9.69 \times 10^{-7}$ |
| BNNR12O-2H-C$_3$H$_6$ | (IM17) | $1.86 \times 10^{-8}$ | $8.32 \times 10^{-9}$ | $5.55 \times 10^{-9}$ |
| BNNR12O-2H | (IM18) | $1.87 \times 10^{-1}$ | $7.46 \times 10^{-2}$ | $4.73 \times 10^{-2}$ |
| BNNR12O-2Hr | (IM19) | $1.19 \times 10^{-8}$ | $1.39 \times 10^{-8}$ | $1.44 \times 10^{-8}$ |
| BNNR11O-H$_2$O | (IM20) | $2.39 \times 10^{-11}$ | $6.79 \times 10^{-11}$ | $1.04 \times 10^{-10}$ |
| BNNR11O | (IM21) | $1.01 \times 10^{-4}$ | $2.89 \times 10^{-4}$ | $4.49 \times 10^{-4}$ |
| BNNR11O-O$_2$ | (IM22′) | $4.42 \times 10^{-8}$ | $9.26 \times 10^{-8}$ | $1.24 \times 10^{-7}$ |

| | | | | |
|---|---|---|---|---|
| BNNR11O-C$_3$H$_8$ | (IM22) | $1.19 \times 10^{-11}$ | $3.83 \times 10^{-11}$ | $6.20 \times 10^{-11}$ |
| BNNR11O-C$_3$H$_7$-H | (IM23) | $2.66 \times 10^{-11}$ | $6.51 \times 10^{-11}$ | $9.33 \times 10^{-11}$ |
| BNNR11O-2H-C$_3$H$_6$ | (IM24) | $5.53 \times 10^{-15}$ | $9.36 \times 10^{-15}$ | $1.13 \times 10^{-14}$ |
| BNNR11O-2H | (IM25) | $1.60 \times 10^{-7}$ | $2.25 \times 10^{-7}$ | $2.50 \times 10^{-7}$ |
| BNNR10O-H$_2$O | (IM26) | $1.94 \times 10^{-17}$ | $2.08 \times 10^{-16}$ | $5.82 \times 10^{-16}$ |
| BNNR10O | (IM27) | $1.00 \times 10^{-11}$ | $1.15 \times 10^{-10}$ | $3.33 \times 10^{-10}$ |
| BNNR10O-O$_2$ | (IM28) | $5.60 \times 10^{-15}$ | $4.71 \times 10^{-14}$ | $1.19 \times 10^{-13}$ |
| BNNR12O-O$_2$ | (IM15′) | $3.30 \times 10^{-4}$ | $2.72 \times 10^{-4}$ | $2.40 \times 10^{-4}$ |

**Table S6:** Selected bond parameters and relative free energies of transition state structures involved in the propane activation on BNNR14O (TS1), $O_2$ dissociation over BNNR12O (TS15′), and the intermediate BNNR12O (IM14) calculated using the PBE, PBE-D3 and SCAN+rvv10 functionals. All structures are fully optimized with the corresponding DFT functional. All free energies are calculated with reference to the sum of the energies of BNNR14O and the reactant gas molecules, $C_3H_8$ and $O_2$. (T = 800 K, $P_{C_3H_8} = 0.3$ atm, $P_{O_2} = 0.15$ atm).

| | Bond lengths (Å) | | Relative free energy (eV) | | |
|---|---|---|---|---|---|
| | TS1 | TS15′ | TS1 | IM14 (12O) | TS15′ |
| **PBE** | C-H = 1.54 <br> N-H = 1.18 | $N_r$-O = 1.30 <br> O-O = 1.64 <br> $N_l$-O = 1.89 | 2.27 | -3.52 | -0.76 |
| **PBE-D3** | C-H = 1.54 <br> N-H = 1.17 | $N_r$-O = 1.30 <br> O-O = 1.64 <br> $N_l$-O = 1.89 | 2.08 | -3.41 | -0.64 |
| **SCAN +rvv10** | C-H = 1.55 <br> N-H = 1.14 | $N_r$-O = 1.29 <br> O-O = 1.66 <br> $N_l$-O = 1.86 | 2.44 | -3.44 | -0.57 |

**Table S7:** ZPE corrected reaction energies ($\Delta E_{ZPE}^{rxn}$), forward activation barriers ($\Delta E_{ZPE}^{act}$), and calculated imaginary vibrational frequency for the corresponding transition state of the elementary steps considered in the overall reaction network of the ODHP reaction. PBE energies are corrected by PBE-D3 single point calculations.

| Reaction | | $\Delta E_{ZPE}^{rxn}$ (eV) | $\Delta E_{ZPE}^{act}$ (eV) | Frequency (i) (cm$^{-1}$) |
|---|---|---|---|---|
| (R1) | BNNR14O (IM0) + $C_3H_{8\,(g)}$ → BNNR14O-$C_3H_8$ (IM1) | -0.14 | - | |
| (R2) | BNNR14O-$C_3H_8$ (IM1) → BNNR14O-$C_3H_7$-H (IM2) | -1.40 | 0.86 | 958 |
| (R3) | BNNR14O-$C_3H_7$-H (IM2) → BNNR14O-2H-$C_3H_6$ (IM3) | 0.44 | 1.36 | 1181 |
| (R4) | BNNR14O-2H-$C_3H_6$ (IM3) → BNNR14O-2H (IM4) + $C_3H_{6\,(g)}$ | 0.09 | - | |
| (R5) | BNNR14O-2H (IM4) → BNNR14O-2Hr (IM5) | 0.93 | 2.05 | 1738 |
| (R6) | BNNR14O-2Hr (IM5) → BNNR13O-$H_2O$ (IM6) | -0.51 | 0.95 | 725 |
| (R7) | BNNR13O-$H_2O$ (IM6) → BNNR13O (IM7) + $H_2O_{(g)}$ | 0.17 | - | |
| (R8) | BNNR13O (IM7) + $C_3H_{8\,(g)}$ → BNNR13O-$C_3H_8$ (IM8) | -0.14 | - | |
| (R9) | BNNR13O-$C_3H_8$ (IM8) → BNNR13O-$C_3H_7$-H (IM9) | -1.39 | 0.88 | 982 |
| (R10) | BNNR13O-$C_3H_7$-H (IM9) → BNNR13O-2H-$C_3H_6$ (IM10) | 0.49 | 1.42 | 1259 |
| (R11) | BNNR13O-2H-$C_3H_6$ (IM10) → BNNR13O-2H (IM11) + $C_3H_{6\,(g)}$ | 0.09 | - | |
| (R12) | BNNR13O-2H (IM11) → BNNR13O-2Hr (IM12) | 0.90 | 1.89 | 1731 |
| (R13) | BNNR13O-2Hr (IM12) → BNNR12O-$H_2O$ (IM13) | -0.65 | 0.89 | 672 |
| (R14) | BNNR12O-$H_2O$ (IM13) → BNNR12O (IM14) + $H_2O_{(g)}$ | 0.25 | - | |
| (R15) | BNNR12O (IM14) + $C_3H_{8\,(g)}$ → BNNR12O- $C_3H_8$ (IM15) | -0.14 | - | |
| (R16) | BNNR12O-$C_3H_8$ (IM15) → BNNR12O-$C_3H_7$-H (IM16) | -1.38 | 0.86 | 853 |
| (R17) | BNNR12O-$C_3H_7$-H (IM16) → BNNR12O-2H-$C_3H_6$ (IM17) | 0.51 | 1.40 | 1394 |
| (R18) | BNNR12O-2H-$C_3H_6$ (IM17) → BNNR12O-2H (IM18) + $C_3H_{6\,(g)}$ | 0.09 | - | |
| (R19) | BNNR12O-2H (IM18) → BNNR12O-2Hr (IM19) | 0.92 | 1.69 | 1721 |
| (R20) | BNNR12O-2Hr (IM19) → BNNR11O-$H_2O$ (IM20) | 0.72 | 1.09 | 2102 |
| (R21) | BNNR11O-$H_2O$ (IM20) → BNNR11O (IM21) + $H_2O_{(g)}$ | 0.01 | - | |
| (R22) | BNNR11O (IM21) + $O_{2\,(g)}$ → BNNR11O-$O_2$ (IM22′) | -0.54 | - | |
| (R23) | BNNR11O-$O_2$ (IM22′) → BNNR13O (IM7) | -2.24 | 0.57 | 521 |
| (R24) | BNNR11O (IM21) + $C_3H_{8\,(g)}$ → BNNR11O- $C_3H_8$ (IM22) | -0.13 | - | |
| (R25) | BNNR11O-$C_3H_8$ (IM22) → BNNR11O-$C_3H_7$-H (IM23) | -1.26 | 0.82 | 842 |
| (R26) | BNNR11O-$C_3H_7$-H (IM23) → BNNR11O-2H-$C_3H_6$ (IM24) | 0.47 | 1.20 | 1335 |
| (R27) | BNNR11O-2H-$C_3H_6$ (IM24) → BNNR11O-2H (IM25) + $C_3H_{6\,(g)}$ | 0.09 | - | |
| (R28) | BNNR11O-2H (IM25) → BNNR10O-$H_2O$ (IM26) | 1.34 | 1.61 | 872 |
| (R29) | BNNR10O-$H_2O$ (IM26) → BNNR10O (IM27) + $H_2O_{(g)}$ | 0.20 | - | |

| | | | |
|---|---|---|---|
| (R30)  BNNR10O (IM27) + $O_{2\,(g)}$ → BNNR10O-$O_2$ (IM28) | -0.61 | - | |
| (R31)  BNNR10O-$O_2$ (IM28) → BNNR12O (IM14) | -3.33 | 0.13 | 509 |
| (R32)  BNNR12O (IM14) + $O_{2\,(g)}$ → BNNR12O-$O_2$ (IM15′) | 0.62 | - | |
| (R33)  BNNR12O-$O_2$ (IM15′) → BNNR14O (IM0) | -2.26 | 0.67 | 472 |

**Table S8:** Forward rate constants ($k_{for}$) and equilibrium constants ($K$) calculated at different temperatures for the elementary steps considered in the overall reaction network of the ODHP reaction based on single point PBE-D3 corrected PBE optimized structures and free energies ($P_{C_3H_8} = 0.3$ atm and $P_{O_2} = 0.15$ atm).

| Reaction | T= 748 K | | T = 798 K | | T = 823 K | |
|---|---|---|---|---|---|---|
| | $k_{for}$ (s$^{-1}$) | $K$ | $k_{for}$ (s$^{-1}$) | $K$ | $k_{for}$ (s$^{-1}$) | $K$ |
| R1 | $3.03\times10^9$ | $5.51\times10^{-7}$ | $2.94\times10^9$ | $6.93\times10^{-7}$ | $2.89\times10^9$ | $7.77\times10^{-7}$ |
| R2 | $2.80\times10^6$ | $1.39\times10^7$ | $6.76\times10^6$ | $3.41\times10^6$ | $1.01\times10^7$ | $1.80\times10^6$ |
| R3 | $2.45\times10^4$ | $7.26\times10^{-2}$ | $1.01\times10^5$ | $1.20\times10^{-1}$ | $1.92\times10^5$ | $1.51\times10^{-1}$ |
| R4 | $4.54\times10^{15}$ | $1.46\times10^6$ | $3.33\times10^{15}$ | $1.11\times10^6$ | $2.87\times10^{15}$ | $9.70\times10^5$ |
| R5 | $2.04\times10^{-1}$ | $1.85\times10^{-6}$ | $1.54$ | $4.57\times10^{-6}$ | $3.85$ | $6.89\times10^{-6}$ |
| R6 | $1.71\times10^6$ | $9.73\times10^2$ | $4.44\times10^6$ | $5.87\times10^2$ | $6.86\times10^6$ | $4.66\times10^2$ |
| R7 | $2.09\times10^{17}$ | $4.42\times10^7$ | $1.90\times10^{17}$ | $4.14\times10^7$ | $1.80\times10^{17}$ | $3.98\times10^7$ |
| R8 | $3.03\times10^9$ | $6.14\times10^{-7}$ | $2.94\times10^9$ | $7.71\times10^{-7}$ | $2.89\times10^9$ | $8.63\times10^{-7}$ |
| R9 | $2.56\times10^6$ | $1.63\times10^7$ | $6.33\times106$ | $4.04\times10^6$ | $9.57\times10^6$ | $2.14\times10^6$ |
| R10 | $8.24\times10^3$ | $2.32\times10^{-2}$ | $3.58\times10^4$ | $4.04\times10^{-2}$ | $6.98\times10^4$ | $5.21\times10^{-2}$ |
| R11 | $5.54\times10^{15}$ | $1.78\times10^6$ | $4.06\times10^{15}$ | $1.35\times10^6$ | $3.50\times10^{15}$ | $1.18\times10^6$ |
| R12 | $2.60$ | $1.21\times10^{-6}$ | $1.67\times10^1$ | $2.89\times10^{-6}$ | $3.89\times10^1$ | $4.28\times10^{-6}$ |
| R13 | $6.58\times10^7$ | $7.92\times10^7$ | $1.69\times10^8$ | $4.69\times10^7$ | $2.61\times10^8$ | $3.70\times10^7$ |
| R14 | $2.73\times10^{13}$ | $5.75\times10^3$ | $2.39\times10^{13}$ | $5.20\times10^3$ | $2.23\times10^{13}$ | $4.93\times10^3$ |
| R15 | $3.03\times10^9$ | $5.46\times10^{-7}$ | $2.94\times10^9$ | $6.91\times10^{-7}$ | $2.89\times10^9$ | $7.75\times10^{-7}$ |
| R16 | $3.24\times10^6$ | $9.16\times10^6$ | $7.88\times10^6$ | $2.29\times10^6$ | $1.18\times10^7$ | $1.22\times10^6$ |
| R17 | $1.19\times10^4$ | $2.74\times10^{-2}$ | $5.08\times10^4$ | $4.86\times10^{-2}$ | $9.85\times10^4$ | $6.32\times10^{-2}$ |
| R18 | $4.82\times10^{15}$ | $1.55\times10^6$ | $3.53\times10^{15}$ | $1.18\times10^6$ | $3.04\times10^{15}$ | $1.03\times10^6$ |
| R19 | $1.12\times10^2$ | $1.21\times10^{-6}$ | $6.24\times10^2$ | $2.97\times10^{-6}$ | $1.36\times10^3$ | $4.47\times10^{-6}$ |
| R20 | $2.34\times10^6$ | $8.55\times10^{-4}$ | $7.16\times10^6$ | $1.85\times10^{-3}$ | $1.19\times10^7$ | $2.64\times10^{-3}$ |
| R21 | $6.70\times10^{16}$ | $1.41\times10^7$ | $4.81\times10^{16}$ | $1.05\times10^7$ | $4.10\times10^{16}$ | $9.06\times10^6$ |
| R22 | $1.78\times10^9$ | $2.51\times10^{-3}$ | $1.72\times10^9$ | $2.03\times10^{-3}$ | $1.69\times10^9$ | $1.85\times10^{-3}$ |
| R23 | $6.75\times10^5$ | $1.01\times10^{12}$ | $1.11\times106$ | $1.05\times10^{11}$ | $1.40\times10^6$ | $3.73\times10^{10}$ |

| R24 | $3.03\times10^9$ | $6.58\times10^{-7}$ | $2.94\times10^9$ | $8.37\times10^{-7}$ | $2.89\times10^9$ | $9.42\times10^{-7}$ |
|-----|------------------|---------------------|------------------|---------------------|------------------|---------------------|
| R25 | $4.09\times10^6$ | $1.04\times10^6$ | $9.59\times10^6$ | $2.90\times10^5$ | $1.41\times10^7$ | $1.62\times10^5$ |
| R26 | $2.08\times10^5$ | $5.38\times10^{-2}$ | $7.33\times10^5$ | $9.23\times10^{-2}$ | $1.30\times10^6$ | $1.18\times10^{-1}$ |
| R27 | $4.60\times10^{15}$ | $1.48\times10^6$ | $3.37\times10^{15}$ | $1.12\times10^6$ | $2.90\times10^{15}$ | $9.81\times10^5$ |
| R28 | $5.71\times10^2$ | $1.49\times10^{-7}$ | $2.94\times10^3$ | $5.98\times10^{-7}$ | $6.21\times10^3$ | $1.12\times10^{-6}$ |
| R29 | $9.65\times10^{14}$ | $2.04\times10^5$ | $8.37\times10^{14}$ | $1.82\times10^5$ | $7.78\times10^{14}$ | $1.72\times10^5$ |
| R30 | $1.78\times10^9$ | $1.11\times10^{-2}$ | $1.72\times10^9$ | $8.32\times10^{-3}$ | $1.69\times10^9$ | $7.35\times10^{-3}$ |
| R31 | $4.53\times10^8$ | $3.16\times10^{19}$ | $4.88\times10^8$ | $1.12\times10^{18}$ | $5.04\times10^8$ | $2.44\times10^{17}$ |
| R32 | $1.78\times10^9$ | $4.49\times10^{-11}$ | $1.72\times10^9$ | $1.11\times10^{-10}$ | $1.69\times10^9$ | $1.69\times10^{-10}$ |
| R33 | $2.59\times10^5$ | $2.71\times10^{12}$ | $4.83\times10^5$ | $2.84\times10^{11}$ | $6.41\times10^5$ | $1.02\times10^{11}$ |

**Table S9:** Surface coverage/probability density ($\theta$) of various intermediates calculated at different temperatures for overall pathway of the ODHP reaction form a microkinetic model based on single point PBE-D3 corrected PBE optimized structures and free energies ($P_{C3H8}$= 0.3, and $P_{O2}$= 0.15 atm).

| Intermediate | | Surface Coverage ($\theta$) | | |
|---|---|---|---|---|
| | | **748 K** | **798 K** | **823 K** |
| BNNR14O | (IM0) | $2.23\times10^{-6}$ | $4.07\times10^{-6}$ | $5.47\times10^{-6}$ |
| BNNR14O-C$_3$H$_8$ | (IM1) | $1.23\times10^{-12}$ | $2.82\times10^{-12}$ | $4.25\times10^{-12}$ |
| BNNR14O-C$_3$H$_7$-H | (IM2) | $3.47\times10^{-10}$ | $3.17\times10^{-10}$ | $3.29\times10^{-10}$ |
| BNNR14O-2H-C$_3$H$_6$ | (IM3) | $1.50\times10^{-11}$ | $1.53\times10^{-11}$ | $1.59\times10^{-11}$1 |
| BNNR14O-2H | (IM4) | $2.19\times10^{-5}$ | $1.70\times10^{-5}$ | $1.54\times10^{-5}$ |
| BNNR14O-2Hr | (IM5) | $9.39\times10^{-12}$ | $2.09\times10^{-11}$ | $2.94\times10^{-11}$ |
| BNNR13O-H$_2$O | (IM6) | $7.18\times10^{-9}$ | $9.74\times10^{-9}$ | $1.08\times10^{-8}$ |
| BNNR13O | (IM7) | $3.17\times10^{-1}$ | $4.03\times10^{-1}$ | $4.31\times10^{-1}$ |
| BNNR13O-C$_3$H$_8$ | (IM8) | $1.95\times10^{-7}$ | $3.11\times10^{-7}$ | $3.72\times10^{-7}$ |
| BNNR13O-C$_3$H$_7$-H | (IM9) | $6.53\times10^{-5}$ | $5.72\times10^{-5}$ | $5.25\times10^{-5}$ |
| BNNR13O-2H-C$_3$H$_6$ | (IM10) | $1.11\times10^{-7}$ | $9.01\times10^{-8}$ | $7.99\times10^{-8}$ |
| BNNR13O-2H | (IM11) | $1.98\times10^{-1}$ | $1.22\times10^{-1}$ | $9.46\times10^{-2}$ |
| BNNR13O-2Hr | (IM12) | $7.57\times10^{-9}$ | $1.16\times10^{-8}$ | $1.36\times10^{-8}$ |
| BNNR12O-H$_2$O | (IM13) | $4.91\times10^{-5}$ | $6.97\times10^{-5}$ | $7.92\times10^{-5}$ |
| BNNR12O | (IM14) | $2.82\times10^{-1}$ | $3.63\times10^{-1}$ | $3.90\times10^{-1}$ |
| BNNR12O-C$_3$H$_8$ | (IM15) | $1.54\times10^{-7}$ | $2.51\times10^{-7}$ | $3.02\times10^{-7}$ |
| BNNR12O-C$_3$H$_7$-H | (IM16) | $4.68\times10^{-5}$ | $4.08\times10^{-5}$ | $3.76\times10^{-5}$ |
| BNNR12O-2H-C$_3$H$_6$ | (IM17) | $1.30\times10^{-7}$ | $9.46\times10^{-8}$ | $8.05\times10^{-8}$ |
| BNNR12O-2H | (IM18) | $2.02\times10^{-1}$ | $1.11\times10^{-1}$ | $8.27\times10^{-2}$ |
| BNNR12O-2Hr | (IM19) | $2.38\times10^{-7}$ | $3.21\times10^{-7}$ | $3.58\times10^{-7}$ |
| BNNR11O-H$_2$O | (IM20) | $2.08\times10^{-11}$ | $8.32\times10^{-11}$ | $1.52\times10^{-10}$ |
| BNNR11O | (IM21) | $2.94\times10^{-4}$ | $8.71\times10^{-4}$ | $1.37\times10^{-3}$ |

| | | | | |
|---|---|---|---|---|
| BNNR11O-$O_2$ | (IM22′) | $7.38 \times 10^{-7}$ | $1.77 \times 10^{-6}$ | $2.55 \times 10^{-6}$ |
| BNNR11O-$C_3H_8$ | (IM22) | $1.93 \times 10^{-10}$ | $7.29 \times 10^{-10}$ | $1.29 \times 10^{-9}$ |
| BNNR11O-$C_3H_7$-H | (IM23) | $3.81 \times 10^{-9}$ | $9.56 \times 10^{-9}$ | $1.41 \times 10^{-8}$ |
| BNNR11O-2H-$C_3H_6$ | (IM24) | $9.37 \times 10^{-13}$ | $2.13 \times 10^{-12}$ | $3.03 \times 10^{-12}$ |
| BNNR11O-2H | (IM25) | $1.39 \times 10^{-6}$ | $2.39 \times 10^{-6}$ | $2.97 \times 10^{-6}$ |
| BNNR10O-$H_2O$ | (IM26) | $7.73 \times 10^{-16}$ | $9.48 \times 10^{-15}$ | $2.88 \times 10^{-14}$ |
| BNNR10O | (IM27) | $1.57 \times 10^{-10}$ | $1.73 \times 10^{-9}$ | $4.95 \times 10^{-9}$ |
| BNNR10O-$O_2$ | (IM28) | $1.74 \times 10^{-12}$ | $1.43 \times 10^{-11}$ | $3.63 \times 10^{-11}$ |
| BNNR12O-$O_2$ | (IM15′) | $1.27 \times 10^{-11}$ | $4.04 \times 10^{-11}$ | $6.61 \times 10^{-11}$ |

**Table S10:** The turnover frequency (TOF), apparent activation energy ($E_{app}$), and reaction orders calculated from a microkinetic reactor analysis of the proposed overall ODHP reaction based on single point PBE-D3 corrected PBE optimized structures and free energies.

| Reaction pathway | TOF ($s^{-1}$) | | | $E_{app}$ (eV) | Rate-limiting step | Reaction order (T= 798 K) | |
|---|---|---|---|---|---|---|---|
| | 748 K | 798 K | 823 K | | | $C_3H_8$ | $O_2$ |
| Overall reaction | $5.0\times10^{-1}$ | 2.0 | 3.6 | 1.42 | $1^{st}$ C-H cleavage of $C_3H_8$ on the catalyst | 0.9 | 0.0 |
| Path I: 14O to 12O cycle | $3.4\times10^{-6}$ | $1.9\times10^{-5}$ | $4.3\times10^{-5}$ | | | | |
| Path II: 13O to 11O cycle | $5.0\times10^{-1}$ | 2.0 | 3.6 | | | | |
| Path III: 12O to 10O cycle | $7.9\times10^{-4}$ | $7.0\times10^{-3}$ | $1.8\times10^{-2}$ | | | | |

Atomic coordinates of intermediate and transition state in Figure 4:

IM0 (14O)
E+ZPE = -1201.66824 eV
1.0
   20.0422000885     0.0000000000     0.0000000000
    0.0000000000   34.7140998840     0.0000000000
    0.0000000000     0.0000000000   15.0721998215
  B  N  O
 64  64  14
Direct
  0.021363714    0.249719673    0.504482438
  0.021351985    0.375394708    0.499941567
  0.021361130    0.500781256    0.494929370
  0.021129109    0.627857210    0.490925028
  0.083847820    0.312637876    0.502678282
  0.083892435    0.438171978    0.498248994
  0.083336977    0.563780997    0.491778053
  0.086703901    0.688824004    0.493066813
  0.146353548    0.249735497    0.504873469
  0.146345661    0.375403279    0.501506136
  0.146325723    0.501128725    0.496666170
  0.146265780    0.625220204    0.485337768
  0.208843121    0.312652684    0.503954766
  0.208789780    0.438220769    0.500971252
  0.209252766    0.563747096    0.495466058
  0.205591087    0.688720159    0.493030051
  0.271338333    0.249739398    0.505362259
  0.271322797    0.375439350    0.503652982
  0.271319157    0.500886310    0.501338841
  0.271343448    0.627498972    0.496081395
  0.333826122    0.312651338    0.505016848
  0.333842015    0.438213241    0.503828947
  0.333412742    0.563800337    0.503256731
  0.337294351    0.688330658    0.486551200
  0.396324284    0.249727585    0.505569037
  0.396312959    0.375400971    0.504697157
  0.396310985    0.501116252    0.504212322
  0.396440625    0.625451465    0.507171982
  0.458825349    0.312631228    0.505030451
  0.458762111    0.438167720    0.503791931
  0.459274059    0.563737041    0.503000377
  0.455776876    0.688395327    0.486305287
  0.521323273    0.249709811    0.505367890
  0.521310140    0.375386741    0.503686422
  0.521289394    0.500765212    0.501117572

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| 0.521459456 | 0.627370951 | 0.495260892 |
| 0.583820959 | 0.312605651 | 0.504020445 |
| 0.583832141 | 0.438115935 | 0.500885611 |
| 0.583366919 | 0.563504626 | 0.494787320 |
| 0.588032225 | 0.687843795 | 0.490368346 |
| 0.646331255 | 0.249692998 | 0.504893053 |
| 0.646312127 | 0.375329681 | 0.501574820 |
| 0.646297138 | 0.500949166 | 0.496288584 |
| 0.646389783 | 0.624758395 | 0.483671043 |
| 0.708834461 | 0.312589663 | 0.502775439 |
| 0.708765751 | 0.438067474 | 0.498168352 |
| 0.709280650 | 0.563519681 | 0.490943979 |
| 0.705108830 | 0.690079376 | 0.491433053 |
| 0.771348040 | 0.249692668 | 0.504497655 |
| 0.771332575 | 0.375341219 | 0.500008637 |
| 0.771305643 | 0.500657191 | 0.494641696 |
| 0.771208621 | 0.627692981 | 0.489526268 |
| 0.833844108 | 0.312593591 | 0.502029790 |
| 0.833871231 | 0.438086320 | 0.497127847 |
| 0.833279580 | 0.563569790 | 0.492858421 |
| 0.837462915 | 0.688018024 | 0.490053053 |
| 0.896362208 | 0.249700772 | 0.504333966 |
| 0.896347267 | 0.375338527 | 0.499482358 |
| 0.896322238 | 0.501010869 | 0.494802158 |
| 0.896265233 | 0.624851636 | 0.495804477 |
| 0.958856706 | 0.312613206 | 0.501984960 |
| 0.958807791 | 0.438135742 | 0.497155245 |
| 0.959302943 | 0.563629679 | 0.493275932 |
| 0.954804892 | 0.690225583 | 0.490232592 |
| 0.021358810 | 0.291642404 | 0.502981964 |
| 0.021358788 | 0.417240104 | 0.498304707 |
| 0.021373018 | 0.542574290 | 0.493123632 |
| 0.020977857 | 0.671439622 | 0.491653183 |
| 0.083850794 | 0.354449922 | 0.501273447 |
| 0.083941726 | 0.480027072 | 0.496362773 |
| 0.082816868 | 0.605695129 | 0.488419230 |
| 0.110954036 | 0.729046450 | 0.513530961 |
| 0.146350514 | 0.291663778 | 0.503812021 |
| 0.146357176 | 0.417240708 | 0.500152047 |
| 0.146330351 | 0.543079834 | 0.494010414 |
| 0.146233257 | 0.665997589 | 0.481670011 |
| 0.208845643 | 0.354470086 | 0.503094908 |
| 0.208770771 | 0.480097786 | 0.499612037 |
| 0.209746229 | 0.605647162 | 0.491552482 |
| 0.182479205 | 0.728563928 | 0.515601404 |
| 0.271336787 | 0.291668393 | 0.504897608 |

| | | |
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| 0.271317087 | 0.417301230 | 0.503019865 |
| 0.271345637 | 0.542728629 | 0.500361926 |
| 0.271462621 | 0.671094076 | 0.491768404 |
| 0.333813037 | 0.354471570 | 0.504688552 |
| 0.333874633 | 0.480094269 | 0.503682025 |
| 0.333025604 | 0.605774139 | 0.503852200 |
| 0.360912948 | 0.726327467 | 0.450147735 |
| 0.396322309 | 0.291659739 | 0.505350711 |
| 0.396297923 | 0.417244197 | 0.504502717 |
| 0.396337393 | 0.543096702 | 0.504830601 |
| 0.396606691 | 0.666384508 | 0.505737535 |
| 0.458813120 | 0.354449290 | 0.504709495 |
| 0.458724329 | 0.480041687 | 0.503601984 |
| 0.459801425 | 0.605718535 | 0.503481922 |
| 0.432255635 | 0.726387796 | 0.450427816 |
| 0.521319466 | 0.291638009 | 0.504919722 |
| 0.521292201 | 0.417240681 | 0.502995062 |
| 0.521281067 | 0.542597477 | 0.499989497 |
| 0.521745004 | 0.671089186 | 0.490940499 |
| 0.583800356 | 0.354418328 | 0.503177512 |
| 0.583839755 | 0.479977952 | 0.499378241 |
| 0.582919779 | 0.605409033 | 0.490466610 |
| 0.618500821 | 0.728969418 | 0.513286756 |
| 0.646324641 | 0.291620289 | 0.503888234 |
| 0.646285575 | 0.417157632 | 0.500130597 |
| 0.646278390 | 0.542879562 | 0.493353949 |
| 0.646333825 | 0.665570121 | 0.479508992 |
| 0.708825610 | 0.354397889 | 0.501379905 |
| 0.708712981 | 0.479908887 | 0.496100788 |
| 0.709712706 | 0.605384582 | 0.487011517 |
| 0.684081668 | 0.729610620 | 0.511639424 |
| 0.771340950 | 0.291613723 | 0.503051471 |
| 0.771320584 | 0.417178127 | 0.498310402 |
| 0.771278806 | 0.542440500 | 0.492601719 |
| 0.771248448 | 0.671368908 | 0.489599191 |
| 0.833837542 | 0.354398631 | 0.500403750 |
| 0.833898163 | 0.479932733 | 0.495426986 |
| 0.832718002 | 0.605497164 | 0.492910084 |
| 0.868367612 | 0.729949353 | 0.476123183 |
| 0.896355927 | 0.291623970 | 0.502694891 |
| 0.896347933 | 0.417165077 | 0.497822846 |
| 0.896287693 | 0.542956154 | 0.493778958 |
| 0.896026175 | 0.665595011 | 0.497465729 |
| 0.958862797 | 0.354419839 | 0.500351074 |
| 0.958777052 | 0.479989820 | 0.495539202 |
| 0.959722627 | 0.605499911 | 0.493619888 |

| | | |
|---|---|---|
| 0.933990998 | 0.730326657 | 0.476914105 |
| 0.083863207 | 0.230835223 | 0.505231314 |
| 0.208848498 | 0.230845828 | 0.505472482 |
| 0.333826312 | 0.230840580 | 0.505649458 |
| 0.458815404 | 0.230828548 | 0.505656672 |
| 0.583819103 | 0.230811982 | 0.505458846 |
| 0.708838125 | 0.230804674 | 0.505228530 |
| 0.833856861 | 0.230808026 | 0.505073383 |
| 0.958870315 | 0.230821185 | 0.505089454 |
| 0.833318027 | 0.758936145 | 0.462478804 |
| 0.463676753 | 0.753447190 | 0.414961751 |
| 0.214029583 | 0.757820827 | 0.539792944 |
| 0.583204993 | 0.756710069 | 0.536391665 |
| 0.329556114 | 0.753260653 | 0.414323603 |
| 0.080271940 | 0.758975320 | 0.534602537 |

IM1
E+ZPE = -1255.95902 eV
1.0
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     0.0000000000      0.0000000000      15.0721998215
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  64  64  14   8   3
Direct
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| | | |
|---|---|---|
| 0.021365409 | 0.249719646 | 0.504485918 |
| 0.021349035 | 0.375395532 | 0.499941503 |
| 0.021355911 | 0.500778948 | 0.494930002 |
| 0.021124910 | 0.627851331 | 0.490931451 |
| 0.083849242 | 0.312638069 | 0.502681731 |
| 0.083886981 | 0.438171374 | 0.498248140 |
| 0.083334438 | 0.563777755 | 0.491782514 |
| 0.086709284 | 0.688824993 | 0.493072760 |
| 0.146354143 | 0.249734536 | 0.504874355 |
| 0.146346375 | 0.375404350 | 0.501505092 |
| 0.146326901 | 0.501127351 | 0.496670916 |
| 0.146268861 | 0.625216413 | 0.485342102 |
| 0.208841027 | 0.312653316 | 0.503955051 |
| 0.208792374 | 0.438221373 | 0.500970840 |
| 0.209251291 | 0.563745118 | 0.495467228 |
| 0.205593561 | 0.688713236 | 0.493027646 |
| 0.271336620 | 0.249737475 | 0.505362259 |
| 0.271322845 | 0.375442317 | 0.503653868 |
| 0.271318205 | 0.500885540 | 0.501342542 |
| 0.271344995 | 0.627497104 | 0.496082439 |

| | | |
|---|---|---|
| 0.333825051 | 0.312650926 | 0.505018841 |
| 0.333842895 | 0.438210824 | 0.503824517 |
| 0.333414574 | 0.563799623 | 0.503256667 |
| 0.337298681 | 0.688330053 | 0.486554364 |
| 0.396324570 | 0.249725442 | 0.505569575 |
| 0.396312436 | 0.375398306 | 0.504697790 |
| 0.396311675 | 0.501115153 | 0.504207197 |
| 0.396441601 | 0.625451245 | 0.507173881 |
| 0.458827442 | 0.312628756 | 0.505033299 |
| 0.458761111 | 0.438165357 | 0.503787819 |
| 0.459273155 | 0.563737371 | 0.502997530 |
| 0.455776353 | 0.688393789 | 0.486307090 |
| 0.521322321 | 0.249707283 | 0.505369377 |
| 0.521309617 | 0.375385614 | 0.503687561 |
| 0.521289869 | 0.500764827 | 0.501116212 |
| 0.521457030 | 0.627370237 | 0.495262253 |
| 0.583821911 | 0.312602465 | 0.504020856 |
| 0.583833616 | 0.438112775 | 0.500884883 |
| 0.583367966 | 0.563504021 | 0.494790484 |
| 0.588032178 | 0.687844839 | 0.490369643 |
| 0.646334300 | 0.249690415 | 0.504893654 |
| 0.646310889 | 0.375329846 | 0.501574472 |
| 0.646298470 | 0.500949221 | 0.496291242 |
| 0.646391210 | 0.624759659 | 0.483672910 |
| 0.708834984 | 0.312589388 | 0.502774711 |
| 0.708764323 | 0.438067693 | 0.498169016 |
| 0.709279936 | 0.563521439 | 0.490945339 |
| 0.705103501 | 0.690083222 | 0.491435837 |
| 0.771347945 | 0.249689591 | 0.504496706 |
| 0.771330767 | 0.375340999 | 0.500008890 |
| 0.771300742 | 0.500656367 | 0.494643183 |
| 0.771210191 | 0.627692706 | 0.489528324 |
| 0.833840968 | 0.312591833 | 0.502031625 |
| 0.833870755 | 0.438083957 | 0.497131106 |
| 0.833279009 | 0.563568526 | 0.492856301 |
| 0.837457871 | 0.688011925 | 0.490064031 |
| 0.896363255 | 0.249700113 | 0.504335041 |
| 0.896348504 | 0.375339571 | 0.499481314 |
| 0.896322809 | 0.501010264 | 0.494802791 |
| 0.896268564 | 0.624851032 | 0.495808052 |
| 0.958856611 | 0.312612492 | 0.501982461 |
| 0.958806078 | 0.438133737 | 0.497155181 |
| 0.959305131 | 0.563628690 | 0.493277830 |
| 0.954818025 | 0.690215968 | 0.490242653 |
| 0.021359198 | 0.291643421 | 0.502982977 |
| 0.021355233 | 0.417241066 | 0.498304327 |

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| 0.021370080 | 0.542574565 | 0.493123632 |
| 0.020978269 | 0.671440940 | 0.491653594 |
| 0.083849902 | 0.354451213 | 0.501274238 |
| 0.083940328 | 0.480027622 | 0.496363500 |
| 0.082817278 | 0.605696008 | 0.488420116 |
| 0.110964266 | 0.729047769 | 0.513526500 |
| 0.146351633 | 0.291664245 | 0.503815343 |
| 0.146355166 | 0.417243950 | 0.500148472 |
| 0.146327520 | 0.543078736 | 0.494012945 |
| 0.146236017 | 0.665995721 | 0.481674187 |
| 0.208845120 | 0.354472559 | 0.503092820 |
| 0.208769629 | 0.480098335 | 0.499612860 |
| 0.209747751 | 0.605647766 | 0.491551945 |
| 0.182460885 | 0.728567499 | 0.515602638 |
| 0.271334764 | 0.291667569 | 0.504897165 |
| 0.271317920 | 0.417303840 | 0.503017018 |
| 0.271345946 | 0.542728190 | 0.500363761 |
| 0.271463644 | 0.671093251 | 0.491770429 |
| 0.333808278 | 0.354472256 | 0.504694942 |
| 0.333871850 | 0.480092841 | 0.503679462 |
| 0.333026318 | 0.605774853 | 0.503851820 |
| 0.360911425 | 0.726326423 | 0.450147134 |
| 0.396322000 | 0.291659107 | 0.505353875 |
| 0.396297733 | 0.417245022 | 0.504503255 |
| 0.396338012 | 0.543097691 | 0.504826014 |
| 0.396608238 | 0.666384673 | 0.505741015 |
| 0.458815499 | 0.354449097 | 0.504707502 |
| 0.458725091 | 0.480040479 | 0.503596416 |
| 0.459801473 | 0.605719414 | 0.503482396 |
| 0.432256586 | 0.726387357 | 0.450425570 |
| 0.521318895 | 0.291635454 | 0.504923392 |
| 0.521289061 | 0.417240626 | 0.502993512 |
| 0.521281019 | 0.542598411 | 0.499992629 |
| 0.521746051 | 0.671094076 | 0.490941005 |
| 0.583798452 | 0.354419015 | 0.503179315 |
| 0.583843038 | 0.479979875 | 0.499372230 |
| 0.582920445 | 0.605410296 | 0.490467211 |
| 0.618496776 | 0.728973100 | 0.513289635 |
| 0.646325783 | 0.291619025 | 0.503888677 |
| 0.646290619 | 0.417159500 | 0.500129806 |
| 0.646282910 | 0.542881210 | 0.493353601 |
| 0.646336489 | 0.665572813 | 0.479512915 |
| 0.708823660 | 0.354400142 | 0.501378956 |
| 0.708712219 | 0.479910810 | 0.496102085 |
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| 0.684083096 | 0.729612928 | 0.511631831 |

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0.771338999      0.291611360      0.503052641
0.771318396      0.417179830      0.498313281
0.771275523      0.542441929      0.492601814
0.771246497      0.671373963      0.489595489
0.833838018      0.354398933      0.500403876
0.833896831      0.479934656      0.495430403
0.832723236      0.605499801      0.492908502
0.868358285      0.729940123      0.476127169
0.896355642      0.291622542      0.502698530
0.896351930      0.417165517      0.497825250
0.896289501      0.542958902      0.493778009
0.896036833      0.665598967      0.497462660
0.958862987      0.354420526      0.500351201
0.958777813      0.479988611      0.495541258
0.959719868      0.605500680      0.493623558
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0.333826907      0.230840938      0.505648003
0.458815261      0.230826954      0.505660658
0.583820721      0.230811020      0.505458340
0.708839552      0.230807531      0.505226031
0.833859050      0.230809784      0.505066581
0.958874312      0.230824070      0.505090403
0.833313745      0.758936694      0.462449065
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0.214025016      0.757817090      0.539787313
0.583205802      0.756711772      0.536390653
0.329553331      0.753258291      0.414323477
0.080254905      0.758979661      0.534602600
0.934224537      0.813293172      0.559661212
0.817953851      0.838635330      0.544971077
0.839418874      0.880171719      0.608239176
0.875500826      0.872753498      0.501971673
0.017170186      0.845481249      0.659275831
0.995527835      0.876843347      0.570856929
0.960792110      0.884316787      0.677909059
0.899097963      0.821014247      0.665411801
0.917075415      0.836015577      0.605386796
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TS1
E+ZPE = -1254.95851 eV
1.0

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     0.015327554         0.504633085         0.499054817
     0.015190103         0.631479810         0.484819620
     0.077856290         0.316536518         0.507944049
     0.077881122         0.442056664         0.505297909
     0.077336608         0.567477827         0.493809615
     0.080939635         0.692172432         0.475557611
     0.140368661         0.253639496         0.508266080
     0.140354006         0.379299750         0.508721398
     0.140323838         0.504952147         0.503122337
     0.140424429         0.628550335         0.483209398
     0.202857783         0.316552644         0.509643961
     0.202803395         0.442097625         0.508836461
     0.203330737         0.567457552         0.498631358
     0.199854752         0.692180399         0.475256554
     0.265352614         0.253643809         0.508852786
     0.265346404         0.379331151         0.510870648
     0.265374359         0.504742204         0.507685892
     0.265449684         0.631185692         0.490566171
     0.327844114         0.316551188         0.510382840
     0.327892245         0.442096498         0.511080211
     0.327501562         0.567692055         0.504753660
     0.331566771         0.691405736         0.468752648
     0.390331546         0.253631611         0.508882525
     0.390349890         0.379293349         0.511105046
     0.390372896         0.505015498         0.509064721
     0.390535203         0.629401700         0.500727521
     0.452842794         0.316528523         0.509751020
     0.452823380         0.442061938         0.509618999
     0.453323766         0.567599914         0.502656105
     0.449885681         0.691478428         0.469889645
     0.515330678         0.253606941         0.508376904
     0.515350139         0.379285300         0.508908435
     0.515334485         0.504626271         0.504006334
     0.515443070         0.630958717         0.487325702
     0.577835264         0.316501710         0.507980811
     0.577885702         0.441998835         0.505051838
     0.577375228         0.567219093         0.492267128
     0.581806186         0.691262881         0.475203183
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| | | |
|---|---|---|
| 0.640342514 | 0.253592848 | 0.507546310 |
| 0.640351222 | 0.379230795 | 0.505776291 |
| 0.640345274 | 0.504783358 | 0.497265721 |
| 0.640279752 | 0.628221382 | 0.474495277 |
| 0.702850003 | 0.316491161 | 0.506205666 |
| 0.702817313 | 0.441960758 | 0.501243772 |
| 0.703297619 | 0.567273488 | 0.486489477 |
| 0.698749320 | 0.693616263 | 0.477037014 |
| 0.765358871 | 0.253590046 | 0.507007249 |
| 0.765362011 | 0.379245904 | 0.503883963 |
| 0.765367388 | 0.504549569 | 0.494648561 |
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| 0.827312632 | 0.567512717 | 0.487620495 |
| 0.830752811 | 0.692572592 | 0.478668622 |
| 0.890367376 | 0.253597436 | 0.507031198 |
| 0.890368614 | 0.379237910 | 0.504066286 |
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| 0.890316082 | 0.628909452 | 0.484373034 |
| 0.952865681 | 0.316509925 | 0.506319875 |
| 0.952809628 | 0.442032461 | 0.502039123 |
| 0.953282226 | 0.567480299 | 0.490867481 |
| 0.948966038 | 0.693737526 | 0.479829980 |
| 0.015370294 | 0.295526952 | 0.507213838 |
| 0.015356300 | 0.421122812 | 0.504646601 |
| 0.015335362 | 0.546378757 | 0.494885489 |
| 0.015269261 | 0.675102716 | 0.480708346 |
| 0.077863011 | 0.358337986 | 0.507727874 |
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| 0.076905521 | 0.609295641 | 0.487288561 |
| 0.104965117 | 0.733121519 | 0.475580389 |
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| 0.140354577 | 0.421124762 | 0.507956102 |
| 0.140348355 | 0.546854301 | 0.498736930 |
| 0.140550513 | 0.669086788 | 0.473491407 |
| 0.202859067 | 0.358356365 | 0.510083207 |
| 0.202787502 | 0.483957691 | 0.507060336 |
| 0.203872211 | 0.609239048 | 0.491000071 |
| 0.175935773 | 0.733268056 | 0.481607529 |
| 0.265352209 | 0.295556787 | 0.509828815 |
| 0.265342883 | 0.421179157 | 0.510832241 |
| 0.265426392 | 0.546555458 | 0.504620501 |
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| 0.452845506 | 0.358332986 | 0.510288119 |
| 0.452771276 | 0.483918956 | 0.508520251 |
| 0.453793651 | 0.609531683 | 0.499063296 |
| 0.426611112 | 0.727973000 | 0.426335678 |
| 0.515328584 | 0.295522090 | 0.508862846 |
| 0.515341717 | 0.421120669 | 0.508294933 |
| 0.515296799 | 0.546404086 | 0.500364077 |
| 0.515590863 | 0.674385471 | 0.477553644 |
| 0.577832980 | 0.358301805 | 0.507716421 |
| 0.577884512 | 0.483824616 | 0.502320754 |
| 0.576846197 | 0.608944271 | 0.484067928 |
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| 0.640339326 | 0.295505826 | 0.507187738 |
| 0.640337803 | 0.421035148 | 0.504092925 |
| 0.640307588 | 0.546610732 | 0.491552387 |
| 0.640048878 | 0.668851626 | 0.466480330 |
| 0.702857473 | 0.358284031 | 0.505265165 |
| 0.702784909 | 0.483757474 | 0.497644920 |
| 0.703671100 | 0.608964601 | 0.478769544 |
| 0.677055754 | 0.733404098 | 0.493668799 |
| 0.765355683 | 0.295499123 | 0.506117209 |
| 0.765368388 | 0.421056988 | 0.501787546 |
| 0.765362916 | 0.546253813 | 0.489463469 |
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| 0.952879385 | 0.358304910 | 0.505459352 |
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| 0.589282858 | 0.689732841 | 0.492171141 |
| 0.647786400 | 0.251809185 | 0.498749679 |
| 0.647742671 | 0.377422846 | 0.501676754 |
| 0.647738532 | 0.503009200 | 0.500459083 |
| 0.647598494 | 0.626580904 | 0.487350284 |
| 0.710267290 | 0.314701537 | 0.499371186 |
| 0.710227605 | 0.440191875 | 0.500045589 |
| 0.710686308 | 0.565629879 | 0.494129020 |
| 0.706543848 | 0.691619580 | 0.491852020 |
| 0.772791385 | 0.251811300 | 0.497933543 |
| 0.772749464 | 0.377474576 | 0.499344579 |
| 0.772775159 | 0.502853817 | 0.497294099 |
| 0.772464297 | 0.630109275 | 0.490844196 |
| 0.835266659 | 0.314719970 | 0.498721206 |
| 0.835313291 | 0.440243880 | 0.498854745 |
| 0.834724876 | 0.565948117 | 0.494957400 |
| 0.838323982 | 0.691766722 | 0.492909830 |
| 0.897785710 | 0.251818965 | 0.498180975 |
| 0.897758588 | 0.377463560 | 0.499703025 |
| 0.897743456 | 0.503212605 | 0.497964136 |
| 0.897569111 | 0.627548312 | 0.496595747 |
| 0.960277163 | 0.314717003 | 0.499996204 |
| 0.960213306 | 0.440259402 | 0.500608029 |
| 0.960666014 | 0.565840151 | 0.496696858 |
| 0.957056725 | 0.691655459 | 0.490989694 |
| 0.022775144 | 0.293712410 | 0.500503659 |
| 0.022763085 | 0.419294973 | 0.502443979 |
| 0.022802070 | 0.544597127 | 0.498696466 |
| 0.023549607 | 0.672778894 | 0.492731873 |
| 0.085247370 | 0.356484241 | 0.503516659 |
| 0.085378415 | 0.482028316 | 0.503896523 |
| 0.084700906 | 0.607357694 | 0.494845754 |
| 0.111237751 | 0.731076045 | 0.502140645 |
| 0.147775516 | 0.293699636 | 0.502424112 |
| 0.147779608 | 0.419222913 | 0.506772694 |
| 0.147960543 | 0.544921739 | 0.503435004 |
| 0.148430845 | 0.667461311 | 0.487949771 |
| 0.210268432 | 0.356459297 | 0.506403618 |
| 0.210272857 | 0.482005678 | 0.509527917 |
| 0.211535076 | 0.607415386 | 0.501114978 |
| 0.181886317 | 0.731540106 | 0.508629967 |
| 0.272772280 | 0.293678098 | 0.503661999 |
| 0.272784271 | 0.419225935 | 0.510368824 |

| | | |
|---|---|---|
| 0.272938584 | 0.544604160 | 0.511246621 |
| 0.272909796 | 0.673157956 | 0.496405135 |
| 0.335274249 | 0.356431687 | 0.507726260 |
| 0.335389258 | 0.481996942 | 0.513470471 |
| 0.334523551 | 0.607794118 | 0.512833653 |
| 0.362443084 | 0.727518554 | 0.449473933 |
| 0.397772815 | 0.293674938 | 0.503720116 |
| 0.397782356 | 0.419181403 | 0.510675544 |
| 0.397815141 | 0.545054594 | 0.514689440 |
| 0.398014515 | 0.668423059 | 0.509952483 |
| 0.460275974 | 0.356441357 | 0.506395867 |
| 0.460199317 | 0.481991063 | 0.511381679 |
| 0.461198709 | 0.607695658 | 0.510929272 |
| 0.433565936 | 0.727581191 | 0.449703521 |
| 0.522762478 | 0.293679004 | 0.502204109 |
| 0.522755959 | 0.419233875 | 0.507013260 |
| 0.522662648 | 0.544548226 | 0.507410113 |
| 0.522944674 | 0.672940870 | 0.494185302 |
| 0.585236848 | 0.356461934 | 0.503078583 |
| 0.585279483 | 0.481990404 | 0.504406383 |
| 0.584109171 | 0.607279838 | 0.495643730 |
| 0.619731373 | 0.731112858 | 0.511545589 |
| 0.647763275 | 0.293704224 | 0.499852509 |
| 0.647739578 | 0.419222611 | 0.501975311 |
| 0.647637227 | 0.544885256 | 0.497850338 |
| 0.647201126 | 0.667338674 | 0.482314581 |
| 0.710244022 | 0.356484269 | 0.499950963 |
| 0.710169744 | 0.482000843 | 0.499009418 |
| 0.710940261 | 0.607382254 | 0.489665059 |
| 0.685187362 | 0.731661479 | 0.508943141 |
| 0.772773493 | 0.293707850 | 0.498411893 |
| 0.772764167 | 0.419281924 | 0.499192501 |
| 0.772741898 | 0.544588226 | 0.495177340 |
| 0.771799748 | 0.673326855 | 0.490673136 |
| 0.835250957 | 0.356500560 | 0.499025331 |
| 0.835343459 | 0.482055074 | 0.497944932 |
| 0.834121329 | 0.607802470 | 0.494106463 |
| 0.862839668 | 0.730966486 | 0.488689947 |
| 0.897775147 | 0.293720460 | 0.498853417 |
| 0.897769247 | 0.419260880 | 0.499593688 |
| 0.897699489 | 0.545115803 | 0.496521368 |
| 0.897565114 | 0.668208171 | 0.498112608 |
| 0.960264411 | 0.356498115 | 0.500564338 |
| 0.960192846 | 0.482079194 | 0.499771012 |
| 0.961116818 | 0.607665933 | 0.495674513 |
| 0.934347683 | 0.730082154 | 0.480861690 |

| | | |
|---|---|---|
| 0.085282171 | 0.232902757 | 0.498946429 |
| 0.210280827 | 0.232885917 | 0.499471475 |
| 0.335284765 | 0.232879021 | 0.499642883 |
| 0.460278638 | 0.232879241 | 0.499390706 |
| 0.585290665 | 0.232884323 | 0.498622025 |
| 0.710291700 | 0.232900367 | 0.497855052 |
| 0.835287310 | 0.232891164 | 0.497645964 |
| 0.960293056 | 0.232899351 | 0.498138455 |
| 0.832193538 | 0.760287999 | 0.440456825 |
| 0.464995810 | 0.754020316 | 0.411756620 |
| 0.212163842 | 0.762059630 | 0.526408083 |
| 0.584599803 | 0.759388888 | 0.532342020 |
| 0.331051610 | 0.753841856 | 0.411202911 |
| 0.078193037 | 0.761720182 | 0.511714878 |
| 0.958442446 | 0.755626838 | 0.489504343 |
| 0.780262584 | 0.781892669 | 0.548988073 |
| 0.900675255 | 0.796026700 | 0.580468842 |
| 0.906005538 | 0.824359872 | 0.481067835 |
| 0.855598819 | 0.839642628 | 0.571666011 |
| 0.727826342 | 0.801851311 | 0.408757540 |
| 0.752693715 | 0.843590060 | 0.468759165 |
| 0.801315203 | 0.827736156 | 0.376629575 |
| 0.812317322 | 0.793374639 | 0.495816499 |
| 0.872466438 | 0.814273382 | 0.534078694 |
| 0.771104889 | 0.818030431 | 0.433359569 |

TS2
E+ZPE = -1255.86286 eV
1.0

| | | |
|---|---|---|
| 20.0422000885 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 34.7140998840 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 15.0721998215 |

B   N   O   H   C
64  64  14  8   3
Direct

| | | |
|---|---|---|
| 0.025415387 | 0.253148924 | 0.509690941 |
| 0.025407292 | 0.378802942 | 0.503227941 |
| 0.025429888 | 0.504142980 | 0.495562265 |
| 0.025548106 | 0.630828773 | 0.486457998 |
| 0.087928452 | 0.316041166 | 0.507333868 |
| 0.087972437 | 0.441535927 | 0.501133391 |
| 0.087593697 | 0.566913437 | 0.491585796 |
| 0.090888432 | 0.691402330 | 0.482367668 |
| 0.150432247 | 0.253147962 | 0.510523497 |
| 0.150426228 | 0.378780085 | 0.505634304 |

| | | |
|---|---|---|
| 0.150501326 | 0.504380889 | 0.498747402 |
| 0.150731486 | 0.628125943 | 0.484176442 |
| 0.212946587 | 0.316043638 | 0.508912042 |
| 0.212928149 | 0.441532548 | 0.503973432 |
| 0.213539713 | 0.566932832 | 0.495925267 |
| 0.209514093 | 0.692199904 | 0.484196120 |
| 0.275432687 | 0.253136204 | 0.511050947 |
| 0.275451459 | 0.378793409 | 0.507293342 |
| 0.275520240 | 0.504153474 | 0.502401396 |
| 0.275513079 | 0.630944266 | 0.492749716 |
| 0.337933609 | 0.316040479 | 0.509441421 |
| 0.338004556 | 0.441538729 | 0.505269057 |
| 0.337563363 | 0.567146017 | 0.501338303 |
| 0.341582773 | 0.691707052 | 0.479186581 |
| 0.400425205 | 0.253140407 | 0.511023106 |
| 0.400452565 | 0.378774371 | 0.506969981 |
| 0.400457323 | 0.504456493 | 0.502788315 |
| 0.400524035 | 0.628793794 | 0.502149345 |
| 0.462933549 | 0.316038968 | 0.508463020 |
| 0.462909567 | 0.441546504 | 0.503284033 |
| 0.463357231 | 0.567069315 | 0.498687007 |
| 0.459951218 | 0.691518702 | 0.480749790 |
| 0.525430807 | 0.253146122 | 0.510403340 |
| 0.525426097 | 0.378795277 | 0.504569344 |
| 0.525401353 | 0.504152375 | 0.497467342 |
| 0.525391884 | 0.630645368 | 0.489037098 |
| 0.587925448 | 0.316040809 | 0.506671614 |
| 0.587943387 | 0.441524389 | 0.498949498 |
| 0.587425015 | 0.566876569 | 0.488331248 |
| 0.591528171 | 0.691220244 | 0.483887787 |
| 0.650420851 | 0.253159528 | 0.509654401 |
| 0.650404625 | 0.378768464 | 0.501849997 |
| 0.650375551 | 0.504356933 | 0.491504774 |
| 0.650270154 | 0.628217481 | 0.475002067 |
| 0.712917014 | 0.316045177 | 0.505294208 |
| 0.712859058 | 0.441523043 | 0.496045518 |
| 0.713284215 | 0.566979755 | 0.484051255 |
| 0.709301872 | 0.692437539 | 0.487427636 |
| 0.775406516 | 0.253157578 | 0.509219900 |
| 0.775413083 | 0.378792475 | 0.500577752 |
| 0.775400283 | 0.504163639 | 0.490657001 |
| 0.775189584 | 0.631173385 | 0.482126152 |
| 0.837909722 | 0.316042649 | 0.504904379 |
| 0.837939224 | 0.441542246 | 0.496212340 |
| 0.837408194 | 0.567172335 | 0.487414222 |
| 0.840737313 | 0.692383968 | 0.484936613 |

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| 0.900407837 | 0.253160572 | 0.509173742 |
| 0.900406504 | 0.378775992 | 0.501206155 |
| 0.900374052 | 0.504476493 | 0.492900719 |
| 0.900445998 | 0.628745333 | 0.489261720 |
| 0.962926222 | 0.316046083 | 0.505682645 |
| 0.962861413 | 0.441552081 | 0.498294393 |
| 0.963361419 | 0.567066018 | 0.490323453 |
| 0.959778585 | 0.692856655 | 0.484643655 |
| 0.025424767 | 0.295034650 | 0.507486105 |
| 0.025416961 | 0.420606553 | 0.500934237 |
| 0.025474989 | 0.545869641 | 0.492484536 |
| 0.026000002 | 0.674099155 | 0.484382968 |
| 0.087910888 | 0.357819503 | 0.505477955 |
| 0.088039654 | 0.483339511 | 0.498536953 |
| 0.087335427 | 0.608680702 | 0.486773544 |
| 0.113391218 | 0.732394273 | 0.489250869 |
| 0.150438385 | 0.295041737 | 0.509036596 |
| 0.150451839 | 0.420573614 | 0.503739699 |
| 0.150612861 | 0.546258428 | 0.495296579 |
| 0.150961897 | 0.668806736 | 0.478096596 |
| 0.212942947 | 0.357823046 | 0.507507681 |
| 0.212953511 | 0.483355555 | 0.501988693 |
| 0.214165791 | 0.608789987 | 0.490902282 |
| 0.184198295 | 0.733070200 | 0.495940927 |
| 0.275438754 | 0.295034705 | 0.510025912 |
| 0.275467185 | 0.420608311 | 0.505844405 |
| 0.275595279 | 0.545949970 | 0.500516187 |
| 0.275496901 | 0.674652885 | 0.485302936 |
| 0.337945291 | 0.357820272 | 0.508227768 |
| 0.338065201 | 0.483373796 | 0.504059959 |
| 0.337109109 | 0.609128225 | 0.500345823 |
| 0.365847195 | 0.729522599 | 0.442483261 |
| 0.400431961 | 0.295039512 | 0.509871493 |
| 0.400464937 | 0.420576828 | 0.505590202 |
| 0.400451233 | 0.546408702 | 0.502218124 |
| 0.400461225 | 0.669683870 | 0.499479763 |
| 0.462948300 | 0.357817937 | 0.506847546 |
| 0.462865934 | 0.483382917 | 0.501618257 |
| 0.463783435 | 0.608984600 | 0.498391202 |
| 0.437138634 | 0.729642928 | 0.445500975 |
| 0.525437136 | 0.295037946 | 0.508565713 |
| 0.525425573 | 0.420605344 | 0.502418702 |
| 0.525350534 | 0.545935794 | 0.494986854 |
| 0.525373184 | 0.674120144 | 0.485157723 |
| 0.587906938 | 0.357811563 | 0.504337952 |
| 0.587932967 | 0.483333192 | 0.495703650 |

| | | |
|---|---|---|
| 0.586859963 | 0.608720922 | 0.482938871 |
| 0.619003824 | 0.730545007 | 0.514493291 |
| 0.650422088 | 0.295040172 | 0.507123515 |
| 0.650392253 | 0.420549164 | 0.498733165 |
| 0.650302273 | 0.546210791 | 0.486919042 |
| 0.649999262 | 0.669083382 | 0.470802463 |
| 0.712912303 | 0.357810574 | 0.502462202 |
| 0.712811046 | 0.483313302 | 0.492247101 |
| 0.713586369 | 0.608745262 | 0.478864328 |
| 0.686263744 | 0.730517424 | 0.515374314 |
| 0.775410037 | 0.295036353 | 0.506349392 |
| 0.775397380 | 0.420584987 | 0.497356392 |
| 0.775370496 | 0.545903542 | 0.487040844 |
| 0.774673638 | 0.674469316 | 0.483892723 |
| 0.837903536 | 0.357806920 | 0.502051398 |
| 0.837958638 | 0.483345115 | 0.493087282 |
| 0.836900575 | 0.609046523 | 0.486004800 |
| 0.864498707 | 0.731747687 | 0.474094406 |
| 0.900416402 | 0.295041380 | 0.506428137 |
| 0.900400318 | 0.420558367 | 0.498467605 |
| 0.900351498 | 0.546367658 | 0.490314753 |
| 0.900499577 | 0.669381126 | 0.491058093 |
| 0.962916990 | 0.357815217 | 0.503276535 |
| 0.962821158 | 0.483361159 | 0.495596022 |
| 0.963879030 | 0.608867624 | 0.488748032 |
| 0.936028516 | 0.731465437 | 0.475819026 |
| 0.087917930 | 0.234231480 | 0.510931423 |
| 0.212929243 | 0.234221535 | 0.511399807 |
| 0.337933181 | 0.234214310 | 0.511580105 |
| 0.462931789 | 0.234222387 | 0.511440207 |
| 0.587936107 | 0.234228238 | 0.510995804 |
| 0.712909877 | 0.234235930 | 0.510624292 |
| 0.837905154 | 0.234235683 | 0.510425391 |
| 0.962907474 | 0.234237194 | 0.510461932 |
| 0.834012078 | 0.763484340 | 0.453620418 |
| 0.469355536 | 0.756875452 | 0.411654022 |
| 0.214046190 | 0.763883072 | 0.512198574 |
| 0.585241892 | 0.757466160 | 0.547163701 |
| 0.335267064 | 0.756481774 | 0.405303490 |
| 0.080046050 | 0.763120663 | 0.496586857 |
| 0.958737177 | 0.757539621 | 0.468893811 |
| 0.844357642 | 0.796415377 | 0.590272917 |
| 0.865051530 | 0.835371737 | 0.454066372 |
| 0.777016260 | 0.840254050 | 0.435925856 |
| 0.816058893 | 0.865879777 | 0.523367875 |
| 0.716870617 | 0.765736240 | 0.540825635 |

| 0.731474412 | 0.787508820 | 0.646229484 |
| 0.697666990 | 0.817357965 | 0.555781204 |
| 0.802383163 | 0.806819062 | 0.550611107 |
| 0.816403301 | 0.838325059 | 0.486540349 |
| 0.737265444 | 0.797752671 | 0.577760600 |

IM3
E+ZPE = -1256.90321 eV
1.0

| 20.0422000885 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 34.7140998840 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 15.0721998215 |

B  N  O  H  C
64  64  14  8  3
Direct

| 0.025091461 | 0.251735532 | 0.505395952 |
| 0.025142325 | 0.377337133 | 0.496943436 |
| 0.025241283 | 0.502614314 | 0.489128656 |
| 0.025352354 | 0.629354667 | 0.486958367 |
| 0.087622682 | 0.314608845 | 0.502345557 |
| 0.087734312 | 0.440048580 | 0.495202396 |
| 0.087412179 | 0.565447848 | 0.488358867 |
| 0.090657123 | 0.690019487 | 0.494906718 |
| 0.150107253 | 0.251727455 | 0.506614446 |
| 0.150156537 | 0.377334715 | 0.501052907 |
| 0.150263980 | 0.502918047 | 0.495246941 |
| 0.150498542 | 0.626812275 | 0.487898931 |
| 0.212633394 | 0.314625603 | 0.505481783 |
| 0.212645980 | 0.440102673 | 0.501499841 |
| 0.213213910 | 0.565494111 | 0.497670514 |
| 0.209054201 | 0.690693106 | 0.498330966 |
| 0.275132294 | 0.251736164 | 0.507885267 |
| 0.275150447 | 0.377395539 | 0.505668472 |
| 0.275182446 | 0.502752664 | 0.504031422 |
| 0.275023233 | 0.629472798 | 0.502048550 |
| 0.337639354 | 0.314651207 | 0.507825600 |
| 0.337703686 | 0.440170172 | 0.506964982 |
| 0.337144202 | 0.565754108 | 0.508846047 |
| 0.340854796 | 0.690383494 | 0.494001650 |
| 0.400144082 | 0.251755861 | 0.508428029 |
| 0.400146890 | 0.377418148 | 0.507874416 |
| 0.400140038 | 0.503139418 | 0.509018531 |
| 0.399952084 | 0.627463148 | 0.514929532 |
| 0.462644766 | 0.314678048 | 0.507933672 |
| 0.462617358 | 0.440236160 | 0.507427165 |

| | | |
|---|---|---|
| 0.463029335 | 0.565861085 | 0.509930432 |
| 0.459179464 | 0.690302451 | 0.494609173 |
| 0.525138360 | 0.251776630 | 0.507951009 |
| 0.525130319 | 0.377465098 | 0.506106959 |
| 0.525131413 | 0.502917003 | 0.505389340 |
| 0.524986617 | 0.629738674 | 0.504482627 |
| 0.587621676 | 0.314686207 | 0.505748387 |
| 0.587644326 | 0.440230858 | 0.502590838 |
| 0.587140133 | 0.565795372 | 0.500388564 |
| 0.590934141 | 0.690833160 | 0.499525447 |
| 0.650120124 | 0.251786905 | 0.506733654 |
| 0.650088196 | 0.377427132 | 0.501678336 |
| 0.650049606 | 0.503116452 | 0.497231743 |
| 0.649971283 | 0.627263370 | 0.491740469 |
| 0.712605534 | 0.314672141 | 0.502629751 |
| 0.712524595 | 0.440180172 | 0.496236036 |
| 0.712920107 | 0.565701856 | 0.490875327 |
| 0.709985930 | 0.691179530 | 0.497152461 |
| 0.775097034 | 0.251778471 | 0.505486244 |
| 0.775076288 | 0.377405319 | 0.497360916 |
| 0.775041457 | 0.502767060 | 0.490333672 |
| 0.775058635 | 0.629596807 | 0.488842627 |
| 0.837595196 | 0.314642938 | 0.500389861 |
| 0.837618703 | 0.440102013 | 0.491899855 |
| 0.837151434 | 0.565617296 | 0.485846615 |
| 0.840945347 | 0.690173056 | 0.496080793 |
| 0.900081701 | 0.251756081 | 0.504927695 |
| 0.900102447 | 0.377336226 | 0.495454668 |
| 0.900118340 | 0.502949146 | 0.487284163 |
| 0.900454088 | 0.626993098 | 0.486030426 |
| 0.962612172 | 0.314615246 | 0.500278120 |
| 0.962599705 | 0.440056492 | 0.491497782 |
| 0.963218954 | 0.565473672 | 0.484948223 |
| 0.959641736 | 0.691258210 | 0.496016919 |
| 0.025109671 | 0.293627137 | 0.502455052 |
| 0.025158658 | 0.419141568 | 0.494107096 |
| 0.025320500 | 0.544366909 | 0.486758422 |
| 0.025611368 | 0.672701971 | 0.492363841 |
| 0.087636808 | 0.356387072 | 0.499905944 |
| 0.087830139 | 0.481865185 | 0.492709569 |
| 0.087101853 | 0.607304892 | 0.486326642 |
| 0.112840381 | 0.730510282 | 0.511200368 |
| 0.150125001 | 0.293631065 | 0.504806937 |
| 0.150194687 | 0.419134151 | 0.499108695 |
| 0.150357719 | 0.544819047 | 0.493050614 |
| 0.150577364 | 0.667604496 | 0.486572365 |

| | | |
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| 0.212658494 | 0.356416055 | 0.504202894 |
| 0.212665965 | 0.481937547 | 0.500237055 |
| 0.213755694 | 0.607378958 | 0.495422747 |
| 0.183612556 | 0.731042364 | 0.517589401 |
| 0.275138170 | 0.293645900 | 0.507304857 |
| 0.275176070 | 0.419225001 | 0.505027762 |
| 0.275212471 | 0.544558336 | 0.504021172 |
| 0.274816959 | 0.673172131 | 0.498631864 |
| 0.337646896 | 0.356449489 | 0.507532168 |
| 0.337740278 | 0.482020294 | 0.507406665 |
| 0.336574320 | 0.607706152 | 0.510558677 |
| 0.364321745 | 0.728292887 | 0.458186156 |
| 0.400148317 | 0.293668290 | 0.508399430 |
| 0.400168873 | 0.419238270 | 0.508030702 |
| 0.400098688 | 0.545089924 | 0.510813133 |
| 0.399788111 | 0.668334159 | 0.513590153 |
| 0.462653189 | 0.356480148 | 0.507720060 |
| 0.462586096 | 0.482096172 | 0.508037093 |
| 0.463398914 | 0.607781536 | 0.511851012 |
| 0.435746489 | 0.728317667 | 0.458767483 |
| 0.525140930 | 0.293685130 | 0.507444218 |
| 0.525137599 | 0.419302336 | 0.505735384 |
| 0.525099152 | 0.544747784 | 0.505821215 |
| 0.524737994 | 0.673221801 | 0.500360312 |
| 0.587604784 | 0.356483527 | 0.504648563 |
| 0.587652939 | 0.482087765 | 0.501835761 |
| 0.586618049 | 0.607745382 | 0.498868286 |
| 0.616496755 | 0.730904124 | 0.516064884 |
| 0.650119601 | 0.293691669 | 0.505044403 |
| 0.650076871 | 0.419247171 | 0.500051252 |
| 0.649974662 | 0.545049540 | 0.495720766 |
| 0.649913470 | 0.668147293 | 0.490455063 |
| 0.712586453 | 0.356458637 | 0.500347974 |
| 0.712454790 | 0.482016942 | 0.494206183 |
| 0.713263135 | 0.607551373 | 0.489396240 |
| 0.686634465 | 0.730093088 | 0.510448992 |
| 0.775099889 | 0.293664636 | 0.502617128 |
| 0.775053876 | 0.419222694 | 0.494754671 |
| 0.775011622 | 0.544550259 | 0.488328686 |
| 0.775135101 | 0.672927134 | 0.493633144 |
| 0.837578257 | 0.356415451 | 0.497321370 |
| 0.837627172 | 0.481929745 | 0.489168898 |
| 0.836778952 | 0.607527253 | 0.485753129 |
| 0.864499849 | 0.730191933 | 0.506195352 |
| 0.900092645 | 0.293641972 | 0.501534989 |
| 0.900103589 | 0.419125936 | 0.492387411 |

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| 0.900132995 | 0.544861959 | 0.485052847 |
| 0.900664311 | 0.667648781 | 0.489968235 |
| 0.962619214 | 0.356387209 | 0.497139142 |
| 0.962595898 | 0.481871174 | 0.488640024 |
| 0.963794236 | 0.607298409 | 0.484759035 |
| 0.935299254 | 0.730117483 | 0.505467293 |
| 0.087593043 | 0.232832428 | 0.507027940 |
| 0.212622021 | 0.232829022 | 0.507832054 |
| 0.337642899 | 0.232841549 | 0.508373740 |
| 0.462648192 | 0.232858335 | 0.508426859 |
| 0.587636808 | 0.232878554 | 0.507904186 |
| 0.712609626 | 0.232873197 | 0.507086405 |
| 0.837578733 | 0.232861466 | 0.506525926 |
| 0.962573915 | 0.232842620 | 0.506471511 |
| 0.832251685 | 0.761458097 | 0.516073236 |
| 0.467232559 | 0.755358764 | 0.423168227 |
| 0.213572665 | 0.761022332 | 0.540193467 |
| 0.586786970 | 0.761296945 | 0.537717756 |
| 0.332984682 | 0.755305907 | 0.422133037 |
| 0.079097720 | 0.760607996 | 0.525916920 |
| 0.958011627 | 0.756194580 | 0.513747262 |
| 0.751644931 | 0.866476145 | 0.578742988 |
| 0.864370518 | 0.839596694 | 0.524846961 |
| 0.865588270 | 0.875271604 | 0.439591209 |
| 0.872288001 | 0.888825916 | 0.553423498 |
| 0.710116165 | 0.755884253 | 0.520275339 |
| 0.678441951 | 0.882133622 | 0.454793260 |
| 0.751661062 | 0.886203416 | 0.379286977 |
| 0.773321273 | 0.871914441 | 0.513103737 |
| 0.847633277 | 0.868844088 | 0.506929043 |
| 0.732402334 | 0.880481606 | 0.445902605 |

IM4
E+ZPE = -1210.35565 eV
1.0
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    20.0422000885      0.0000000000      0.0000000000
     0.0000000000     34.7140998840      0.0000000000
     0.0000000000      0.0000000000     15.0721998215
  B   N   O   H
 64  64  14   2
Direct
  0.022947943    0.251759130    0.500158659
  0.022951813    0.377393726    0.502339736
  0.023046112    0.502667555    0.497697595
  0.023153403    0.629391919    0.489011314
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| 0.085445347 | 0.314657663 | 0.502622949 |
| 0.085528820 | 0.440116079 | 0.503077634 |
| 0.085178999 | 0.565482902 | 0.495088725 |
| 0.088550009 | 0.690114101 | 0.490731980 |
| 0.147961114 | 0.251782949 | 0.500896937 |
| 0.147964778 | 0.377391418 | 0.505247354 |
| 0.148022318 | 0.502985849 | 0.503467274 |
| 0.148280743 | 0.626746012 | 0.490329370 |
| 0.210464523 | 0.314682746 | 0.504215707 |
| 0.210443491 | 0.440174540 | 0.507961449 |
| 0.211012682 | 0.565550209 | 0.503631659 |
| 0.207014256 | 0.690703710 | 0.493421810 |
| 0.272965587 | 0.251809377 | 0.501293062 |
| 0.272964326 | 0.377452654 | 0.507800164 |
| 0.272996041 | 0.502836345 | 0.510880424 |
| 0.272878819 | 0.629519940 | 0.502858770 |
| 0.335449974 | 0.314717003 | 0.504787575 |
| 0.335510619 | 0.440231984 | 0.511479785 |
| 0.335001168 | 0.565881030 | 0.513437632 |
| 0.338754873 | 0.690105365 | 0.487986691 |
| 0.397943830 | 0.251833031 | 0.501124691 |
| 0.397963743 | 0.377464961 | 0.508186355 |
| 0.397968478 | 0.503215736 | 0.514187805 |
| 0.397855872 | 0.627647706 | 0.514949431 |
| 0.460447274 | 0.314732827 | 0.504049297 |
| 0.460420532 | 0.440277781 | 0.510496321 |
| 0.460871860 | 0.565950370 | 0.513185739 |
| 0.456981400 | 0.690002014 | 0.487892540 |
| 0.522926450 | 0.251834102 | 0.500564402 |
| 0.522940915 | 0.377505757 | 0.506053746 |
| 0.522939916 | 0.502958321 | 0.509585021 |
| 0.522836089 | 0.629731037 | 0.503246543 |
| 0.585421329 | 0.314728295 | 0.502448314 |
| 0.585456493 | 0.440267231 | 0.505767053 |
| 0.584962435 | 0.565792405 | 0.503092693 |
| 0.588654615 | 0.690762556 | 0.492489028 |
| 0.647903551 | 0.251812866 | 0.500045304 |
| 0.647912258 | 0.377463697 | 0.502875981 |
| 0.647876571 | 0.503126067 | 0.501771918 |
| 0.647793110 | 0.627151173 | 0.490685790 |
| 0.710416416 | 0.314702553 | 0.500999282 |
| 0.710370974 | 0.440219814 | 0.500855461 |
| 0.710772054 | 0.565664988 | 0.494218648 |
| 0.707704881 | 0.691139695 | 0.490589867 |
| 0.772901588 | 0.251773306 | 0.499799201 |
| 0.772918052 | 0.377449604 | 0.500561839 |

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| 0.772911675 | 0.502792004 | 0.496349074 |
| 0.772873038 | 0.629533292 | 0.488378482 |
| 0.835406078 | 0.314665795 | 0.500414190 |
| 0.835469745 | 0.440160529 | 0.498477697 |
| 0.835020749 | 0.565604439 | 0.490584711 |
| 0.838665916 | 0.690217891 | 0.490479107 |
| 0.897918849 | 0.251758608 | 0.499745861 |
| 0.897927985 | 0.377383698 | 0.500428553 |
| 0.897978613 | 0.502991563 | 0.494926396 |
| 0.898291521 | 0.626980131 | 0.487456805 |
| 0.960426670 | 0.314647389 | 0.501024244 |
| 0.960426765 | 0.440117453 | 0.499514912 |
| 0.961056768 | 0.565487847 | 0.491127757 |
| 0.957390474 | 0.691444527 | 0.491364464 |
| 0.022941897 | 0.293661532 | 0.501263671 |
| 0.022972302 | 0.419207914 | 0.501773594 |
| 0.023111616 | 0.544398722 | 0.494461302 |
| 0.023412704 | 0.672823124 | 0.490081558 |
| 0.085455547 | 0.356442566 | 0.503599706 |
| 0.085606725 | 0.481928207 | 0.501448462 |
| 0.084850662 | 0.607294068 | 0.490609894 |
| 0.110996552 | 0.730907256 | 0.501630596 |
| 0.147963196 | 0.293683510 | 0.502743169 |
| 0.147995113 | 0.419197611 | 0.505684860 |
| 0.148110348 | 0.544875750 | 0.500564623 |
| 0.148385106 | 0.667463948 | 0.485277690 |
| 0.210482866 | 0.356467456 | 0.506050709 |
| 0.210451390 | 0.482017437 | 0.507918011 |
| 0.211542475 | 0.607393298 | 0.498872051 |
| 0.181830478 | 0.731496480 | 0.507508409 |
| 0.272970964 | 0.293706064 | 0.503596131 |
| 0.272988356 | 0.419278682 | 0.509665442 |
| 0.273036034 | 0.544648994 | 0.510326937 |
| 0.272704569 | 0.673098725 | 0.495063795 |
| 0.335465010 | 0.356501302 | 0.507252467 |
| 0.335562318 | 0.482086282 | 0.513320133 |
| 0.334449915 | 0.607853403 | 0.512695906 |
| 0.362112928 | 0.727059438 | 0.447082755 |
| 0.397948707 | 0.293734526 | 0.503442819 |
| 0.397975496 | 0.419280715 | 0.510694621 |
| 0.397947946 | 0.545189428 | 0.515583940 |
| 0.397697586 | 0.668492564 | 0.509970769 |
| 0.460457361 | 0.356522758 | 0.506308929 |
| 0.460397549 | 0.482140402 | 0.512421614 |
| 0.461271179 | 0.607894996 | 0.512841277 |
| 0.433489756 | 0.727101196 | 0.447367139 |

| | | |
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| 0.522928972 | 0.293735899 | 0.502347361 |
| 0.522932303 | 0.419340824 | 0.507792888 |
| 0.522923119 | 0.544789927 | 0.509499380 |
| 0.522549400 | 0.673093286 | 0.495117451 |
| 0.585411717 | 0.356522126 | 0.503885671 |
| 0.585453590 | 0.482120073 | 0.506001418 |
| 0.584475563 | 0.607703625 | 0.499179182 |
| 0.614042217 | 0.731139231 | 0.504757235 |
| 0.647909213 | 0.293720625 | 0.501077425 |
| 0.647898792 | 0.419283517 | 0.503182890 |
| 0.647820756 | 0.545040968 | 0.499535887 |
| 0.647692614 | 0.667975261 | 0.485980566 |
| 0.710409088 | 0.356497181 | 0.501447798 |
| 0.710308687 | 0.482048260 | 0.499552655 |
| 0.711120506 | 0.607471704 | 0.490172261 |
| 0.684227987 | 0.730245944 | 0.499711092 |
| 0.772900113 | 0.293682603 | 0.500371986 |
| 0.772902349 | 0.419270550 | 0.499779966 |
| 0.772894307 | 0.544547457 | 0.493395804 |
| 0.772899446 | 0.672900815 | 0.489184400 |
| 0.835404841 | 0.356457429 | 0.500408717 |
| 0.835496011 | 0.481979030 | 0.496312787 |
| 0.834635609 | 0.607488462 | 0.487902822 |
| 0.862015525 | 0.730452700 | 0.495795809 |
| 0.897913900 | 0.293663867 | 0.500317982 |
| 0.897933599 | 0.419184617 | 0.499419274 |
| 0.897995838 | 0.544878882 | 0.491647045 |
| 0.898472814 | 0.667665539 | 0.487816801 |
| 0.960441897 | 0.356435121 | 0.501337417 |
| 0.960422863 | 0.481928262 | 0.497233008 |
| 0.961625294 | 0.607298684 | 0.488403222 |
| 0.932843955 | 0.730458414 | 0.495835861 |
| 0.085466164 | 0.232865834 | 0.499849978 |
| 0.210477584 | 0.232892070 | 0.500227691 |
| 0.335465201 | 0.232913389 | 0.500211239 |
| 0.460433712 | 0.232926576 | 0.499925179 |
| 0.585403247 | 0.232911054 | 0.499642851 |
| 0.710383964 | 0.232876219 | 0.499555122 |
| 0.835403985 | 0.232852538 | 0.499483845 |
| 0.960435425 | 0.232850505 | 0.499479542 |
| 0.829565988 | 0.761840236 | 0.501058633 |
| 0.464953747 | 0.753146204 | 0.407958836 |
| 0.212001559 | 0.761962048 | 0.525686446 |
| 0.584230652 | 0.761972323 | 0.522617986 |
| 0.330603923 | 0.753042524 | 0.407450020 |
| 0.077434154 | 0.761374911 | 0.512356284 |

|  |  |  |
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| 0.955293001 | 0.756754958 | 0.501176164 |
| 0.707696792 | 0.756152767 | 0.507504170 |

TS4
E+ZPE = -1208.36282 eV
1.0
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| 20.0422000885 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 34.7140998840 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 15.0721998215 |

B   N   O   H
64   64   14   2
Direct
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|---|---|---|
| 0.530783597 | 0.251688939 | 0.501406670 |
| 0.530759377 | 0.377386748 | 0.500526311 |
| 0.530706607 | 0.502827499 | 0.497994223 |
| 0.530594549 | 0.629780762 | 0.492428539 |
| 0.593264058 | 0.314599944 | 0.501901565 |
| 0.593256826 | 0.440146326 | 0.501705575 |
| 0.592740309 | 0.565686856 | 0.497923198 |
| 0.596338464 | 0.690240144 | 0.490506821 |
| 0.655766360 | 0.251679818 | 0.502270040 |
| 0.655734289 | 0.377335237 | 0.503767919 |
| 0.655693700 | 0.503024584 | 0.503374515 |
| 0.655929619 | 0.626947933 | 0.495269086 |
| 0.718253435 | 0.314577362 | 0.504277241 |
| 0.718168214 | 0.440093030 | 0.506363439 |
| 0.718719228 | 0.565528341 | 0.504650524 |
| 0.715499646 | 0.690737007 | 0.493374924 |
| 0.780754786 | 0.251654324 | 0.503294410 |
| 0.780738274 | 0.377315457 | 0.507095326 |
| 0.780745507 | 0.502671896 | 0.508780970 |
| 0.780906243 | 0.629306151 | 0.503887190 |
| 0.843252757 | 0.314537088 | 0.506106421 |
| 0.843281307 | 0.440026355 | 0.509454076 |
| 0.842908920 | 0.565529825 | 0.510199377 |
| 0.846573882 | 0.689959982 | 0.492952034 |
| 0.905763339 | 0.251635560 | 0.503843531 |
| 0.905762768 | 0.377250815 | 0.508325811 |
| 0.905782848 | 0.502882883 | 0.509927807 |
| 0.906085954 | 0.627017273 | 0.510353449 |
| 0.968282009 | 0.314521236 | 0.506168714 |
| 0.968240326 | 0.439988553 | 0.508312650 |
| 0.968768977 | 0.565446199 | 0.506592110 |
| 0.965050817 | 0.690183001 | 0.490643302 |
| 0.030788454 | 0.251625670 | 0.503586039 |

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| 0.030800668 | 0.377267243 | 0.506475877 |
| 0.030757266 | 0.502555413 | 0.504498541 |
| 0.030779942 | 0.629228569 | 0.497091718 |
| 0.093300067 | 0.314525659 | 0.504463139 |
| 0.093322294 | 0.439995284 | 0.503591227 |
| 0.092669017 | 0.565321860 | 0.496026853 |
| 0.097299629 | 0.689796687 | 0.493066053 |
| 0.155807603 | 0.251638362 | 0.502700871 |
| 0.155807282 | 0.377273012 | 0.502937135 |
| 0.155705775 | 0.502859256 | 0.497353228 |
| 0.155458984 | 0.626568542 | 0.484256736 |
| 0.218316341 | 0.314555879 | 0.502108439 |
| 0.218245584 | 0.440057343 | 0.499054184 |
| 0.218555066 | 0.565474056 | 0.489922045 |
| 0.214030273 | 0.691624580 | 0.493040934 |
| 0.280808031 | 0.251657126 | 0.501712440 |
| 0.280810482 | 0.377338726 | 0.500011801 |
| 0.280742081 | 0.502725906 | 0.494091119 |
| 0.280195277 | 0.629826256 | 0.487571362 |
| 0.343301887 | 0.314583351 | 0.500494073 |
| 0.343319112 | 0.440127095 | 0.497117628 |
| 0.342635673 | 0.565798613 | 0.490455949 |
| 0.345425316 | 0.690916071 | 0.491484621 |
| 0.405795505 | 0.251680367 | 0.501191919 |
| 0.405793744 | 0.377354907 | 0.499089080 |
| 0.405703051 | 0.503128814 | 0.494568456 |
| 0.405481312 | 0.627411995 | 0.490851979 |
| 0.468289575 | 0.314596565 | 0.500398814 |
| 0.468208683 | 0.440181738 | 0.498134311 |
| 0.468594774 | 0.565816415 | 0.493314751 |
| 0.465202274 | 0.692011664 | 0.491235291 |
| 0.530784168 | 0.293597054 | 0.501054045 |
| 0.530744912 | 0.419223902 | 0.499985352 |
| 0.530703562 | 0.544612456 | 0.496325188 |
| 0.530889565 | 0.673319273 | 0.491078720 |
| 0.593248737 | 0.356397566 | 0.501954779 |
| 0.593284900 | 0.481993426 | 0.501043732 |
| 0.592396424 | 0.607583516 | 0.495069837 |
| 0.620446693 | 0.731236098 | 0.492382191 |
| 0.655762078 | 0.293593071 | 0.502780722 |
| 0.655716065 | 0.419159150 | 0.504059737 |
| 0.655740665 | 0.544959705 | 0.502140993 |
| 0.656134465 | 0.667644990 | 0.490141795 |
| 0.718244632 | 0.356372677 | 0.505214515 |
| 0.718145136 | 0.481950624 | 0.506559145 |
| 0.719333006 | 0.607403078 | 0.501787736 |

| | | |
|---|---|---|
| 0.691138702 | 0.730367701 | 0.494760619 |
| 0.780747125 | 0.293563950 | 0.504744644 |
| 0.780717623 | 0.419150716 | 0.508108022 |
| 0.780817072 | 0.544486029 | 0.508750789 |
| 0.781269494 | 0.672792135 | 0.497277964 |
| 0.843237340 | 0.356330617 | 0.507613538 |
| 0.843319850 | 0.481880899 | 0.510253065 |
| 0.842627132 | 0.607495660 | 0.510173625 |
| 0.869331840 | 0.728969253 | 0.465847846 |
| 0.905761626 | 0.293541368 | 0.505682835 |
| 0.905756011 | 0.419064508 | 0.509389632 |
| 0.905832049 | 0.544848058 | 0.510319408 |
| 0.906398195 | 0.667968009 | 0.507755208 |
| 0.968283627 | 0.356313474 | 0.507461080 |
| 0.968196359 | 0.481834361 | 0.508339952 |
| 0.969284780 | 0.607429561 | 0.506029955 |
| 0.939389611 | 0.729483479 | 0.460842925 |
| 0.030785819 | 0.293533099 | 0.505005174 |
| 0.030784097 | 0.419093382 | 0.506568731 |
| 0.030685138 | 0.544348063 | 0.502728237 |
| 0.030852953 | 0.673048067 | 0.493378183 |
| 0.093300204 | 0.356319298 | 0.504904916 |
| 0.093297593 | 0.481818483 | 0.501882077 |
| 0.092010708 | 0.607190608 | 0.491480160 |
| 0.127658730 | 0.730664181 | 0.515475046 |
| 0.155811231 | 0.293548786 | 0.503183618 |
| 0.155786916 | 0.419077970 | 0.501930608 |
| 0.155566344 | 0.544735422 | 0.493658232 |
| 0.155044735 | 0.667331477 | 0.481427198 |
| 0.218321432 | 0.356347869 | 0.501691655 |
| 0.218168880 | 0.481872603 | 0.496558447 |
| 0.218761363 | 0.607226706 | 0.485835384 |
| 0.193247035 | 0.731285384 | 0.512807900 |
| 0.280813075 | 0.293567384 | 0.501328337 |
| 0.280795303 | 0.419155551 | 0.498608358 |
| 0.280671562 | 0.544467952 | 0.491066477 |
| 0.279402753 | 0.673126088 | 0.490108861 |
| 0.343304338 | 0.356375534 | 0.499711472 |
| 0.343328058 | 0.481954855 | 0.495008778 |
| 0.342000864 | 0.607691647 | 0.489058896 |
| 0.373372829 | 0.730309459 | 0.490529441 |
| 0.405798931 | 0.293588126 | 0.500500084 |
| 0.405788177 | 0.419168216 | 0.497910005 |
| 0.405642144 | 0.545048880 | 0.492442174 |
| 0.405394520 | 0.668087678 | 0.491804976 |
| 0.468292668 | 0.356392539 | 0.499781864 |

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| 0.468159482    | 0.482023810    | 0.496709481    |
| 0.469028401    | 0.607654504    | 0.491832848    |
| 0.441351138    | 0.731401262    | 0.490511883    |
| 0.593277001    | 0.232771467    | 0.501739205    |
| 0.718255386    | 0.232756220    | 0.502355649    |
| 0.843251901    | 0.232739517    | 0.502891894    |
| 0.968266687    | 0.232728006    | 0.503056754    |
| 0.093295731    | 0.232728611    | 0.502741524    |
| 0.218310964    | 0.232737017    | 0.502158583    |
| 0.343311808    | 0.232755753    | 0.501607248    |
| 0.468295999    | 0.232773390    | 0.501432296    |
| 0.354961108    | 0.767190346    | 0.488552232    |
| 0.969189899    | 0.757792695    | 0.429113142    |
| 0.720852722    | 0.764984270    | 0.504251077    |
| 0.092416641    | 0.758546643    | 0.538922361    |
| 0.836698061    | 0.758478292    | 0.437051654    |
| 0.589438217    | 0.762437703    | 0.494682444    |
| 0.768447409    | 0.762169299    | 0.475497786    |
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Direct
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| 0.530698613    | 0.251615918    | 0.501490824    |
| 0.530693427    | 0.377277216    | 0.500909750    |
| 0.530654837    | 0.502572007    | 0.497943699    |
| 0.530355110    | 0.629359887    | 0.491924184    |
| 0.593188401    | 0.314541703    | 0.502191897    |
| 0.593239077    | 0.440048195    | 0.501879040    |
| 0.592645761    | 0.565518286    | 0.497766754    |
| 0.595694709    | 0.690654865    | 0.492567361    |
| 0.655688895    | 0.251654626    | 0.502431989    |
| 0.655701409    | 0.377313671    | 0.503999343    |
| 0.655672716    | 0.503014914    | 0.503095319    |
| 0.655515739    | 0.627011229    | 0.495345616    |
| 0.718182631    | 0.314582884    | 0.504523502    |
| 0.718145659    | 0.440139568    | 0.506195859    |
| 0.718620017    | 0.565714219    | 0.503938916    |
| 0.714171215    | 0.691269858    | 0.491804913    |

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| 0.780677320 | 0.251685285 | 0.503509636 |
| 0.780691547 | 0.377377050 | 0.507108392 |
| 0.780682364 | 0.502836839 | 0.508032189 |
| 0.780591194 | 0.629804058 | 0.503477524 |
| 0.843158828 | 0.314597884 | 0.506282449 |
| 0.843215071 | 0.440166738 | 0.509011381 |
| 0.842765124 | 0.565832954 | 0.509144415 |
| 0.845930746 | 0.690383054 | 0.493080923 |
| 0.905640764 | 0.251690148 | 0.504073911 |
| 0.905675500 | 0.377353726 | 0.508243333 |
| 0.905697198 | 0.503107056 | 0.509054186 |
| 0.905857934 | 0.627330347 | 0.509389221 |
| 0.968157151 | 0.314583159 | 0.506312251 |
| 0.968134406 | 0.440140777 | 0.507884571 |
| 0.968689322 | 0.565719328 | 0.505733834 |
| 0.964791583 | 0.690596569 | 0.490748115 |
| 0.030624303 | 0.251659543 | 0.503833819 |
| 0.030664258 | 0.377342407 | 0.506431743 |
| 0.030663345 | 0.502750302 | 0.503872384 |
| 0.030786232 | 0.629503072 | 0.496974092 |
| 0.093137249 | 0.314542912 | 0.504610535 |
| 0.093170605 | 0.440075750 | 0.503302098 |
| 0.092682513 | 0.565543506 | 0.495734180 |
| 0.097507842 | 0.689985421 | 0.494002473 |
| 0.155622171 | 0.251622264 | 0.502891894 |
| 0.155627060 | 0.377255787 | 0.502969215 |
| 0.155591706 | 0.502933047 | 0.496974567 |
| 0.155721263 | 0.626839858 | 0.484818101 |
| 0.218144612 | 0.314498434 | 0.502247641 |
| 0.218035528 | 0.439982674 | 0.498874139 |
| 0.218583259 | 0.565525429 | 0.489853994 |
| 0.214736933 | 0.692137322 | 0.493699360 |
| 0.280645154 | 0.251589901 | 0.501845125 |
| 0.280626739 | 0.377228755 | 0.500133508 |
| 0.280530573 | 0.502526952 | 0.493748397 |
| 0.280666352 | 0.629783729 | 0.487470726 |
| 0.343160660 | 0.314477391 | 0.500700250 |
| 0.343134394 | 0.439936328 | 0.497096115 |
| 0.342481027 | 0.565355596 | 0.490031730 |
| 0.347519482 | 0.690299978 | 0.490139327 |
| 0.405674739 | 0.251588280 | 0.501281072 |
| 0.405661035 | 0.377206722 | 0.499388744 |
| 0.405548548 | 0.502792664 | 0.494342569 |
| 0.405507578 | 0.626444147 | 0.489763861 |
| 0.468189983 | 0.314497720 | 0.500682597 |
| 0.468110900 | 0.439971960 | 0.498305371 |

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| 0.465026359 | 0.690889862 | 0.490176089 |
| 0.530699089 | 0.293522412 | 0.501267911 |
| 0.530692095 | 0.419093107 | 0.500283941 |
| 0.530612773 | 0.544281306 | 0.496106040 |
| 0.529697127 | 0.672396700 | 0.490498469 |
| 0.593207291 | 0.356335012 | 0.502315819 |
| 0.593274336 | 0.481863097 | 0.501075938 |
| 0.592112875 | 0.607287145 | 0.495162122 |
| 0.619106033 | 0.729725564 | 0.497580476 |
| 0.655696460 | 0.293566176 | 0.503051344 |
| 0.655722679 | 0.419124370 | 0.504197548 |
| 0.655710735 | 0.544911574 | 0.501753315 |
| 0.655391261 | 0.667569551 | 0.490590911 |
| 0.718217272 | 0.356381358 | 0.505389625 |
| 0.718149418 | 0.481984470 | 0.506127650 |
| 0.719156281 | 0.607567582 | 0.501223334 |
| 0.689291232 | 0.730229076 | 0.491261581 |
| 0.780678985 | 0.293593428 | 0.504994101 |
| 0.780700017 | 0.419217749 | 0.507898207 |
| 0.780764873 | 0.544648225 | 0.507794501 |
| 0.780890065 | 0.673260207 | 0.497350413 |
| 0.843182715 | 0.356399544 | 0.507670231 |
| 0.843288825 | 0.482033425 | 0.509501531 |
| 0.842458687 | 0.607789887 | 0.509240970 |
| 0.869356298 | 0.729841717 | 0.466722985 |
| 0.905656752 | 0.293599774 | 0.505864557 |
| 0.905687491 | 0.419188189 | 0.509044347 |
| 0.905786750 | 0.545095198 | 0.509216199 |
| 0.906142292 | 0.668260753 | 0.506821383 |
| 0.968174471 | 0.356388253 | 0.507494457 |
| 0.968134786 | 0.482015678 | 0.507673490 |
| 0.969294297 | 0.607728130 | 0.505315974 |
| 0.939648369 | 0.729987869 | 0.462259086 |
| 0.030633820 | 0.293572137 | 0.505189585 |
| 0.030653332 | 0.419193710 | 0.506308264 |
| 0.030692103 | 0.544590039 | 0.502036149 |
| 0.031045279 | 0.673395096 | 0.493795631 |
| 0.093130207 | 0.356345671 | 0.504986951 |
| 0.093188889 | 0.481944855 | 0.501436061 |
| 0.092248321 | 0.607501099 | 0.491572192 |
| 0.128323409 | 0.731043353 | 0.517002537 |
| 0.155627726 | 0.293535022 | 0.503330951 |
| 0.155582712 | 0.419076514 | 0.501806212 |
| 0.155577811 | 0.544892288 | 0.493432883 |
| 0.155753334 | 0.667697297 | 0.482513767 |

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| 0.193883938 | 0.731677193 | 0.514181794 |
| 0.280640752 | 0.293499363 | 0.501484876 |
| 0.280569663 | 0.419049591 | 0.498604751 |
| 0.280446208 | 0.544304932 | 0.490736947 |
| 0.280958561 | 0.673655918 | 0.489842257 |
| 0.343133204 | 0.356267843 | 0.499952608 |
| 0.343087167 | 0.481754088 | 0.494763687 |
| 0.341860113 | 0.607298739 | 0.488523442 |
| 0.380332460 | 0.732732951 | 0.488862811 |
| 0.405674548 | 0.293496369 | 0.500692658 |
| 0.405619970 | 0.419006487 | 0.498091759 |
| 0.405409366 | 0.544682126 | 0.492003846 |
| 0.405235545 | 0.667227192 | 0.489993734 |
| 0.468192505 | 0.356286908 | 0.500190391 |
| 0.468023917 | 0.481782329 | 0.496701762 |
| 0.468744804 | 0.607017093 | 0.491026393 |
| 0.446381075 | 0.731778565 | 0.489868737 |
| 0.593210004 | 0.232722841 | 0.501798461 |
| 0.718200380 | 0.232766632 | 0.502509721 |
| 0.843168059 | 0.232777319 | 0.503108512 |
| 0.968124128 | 0.232772346 | 0.503333387 |
| 0.093104268 | 0.232739737 | 0.503005977 |
| 0.218115253 | 0.232701853 | 0.502321671 |
| 0.343152142 | 0.232687210 | 0.501688554 |
| 0.468193504 | 0.232695644 | 0.501448937 |
| 0.347199817 | 0.762973082 | 0.486378178 |
| 0.970090175 | 0.758526973 | 0.432211499 |
| 0.719584721 | 0.763067861 | 0.525335972 |
| 0.093372209 | 0.758794718 | 0.541092081 |
| 0.837358327 | 0.759400811 | 0.439905932 |
| 0.588088945 | 0.763912138 | 0.470227653 |
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 64  64  14  2

Direct
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| 0.032296072 | 0.503391009 | 0.504224123 |
| 0.032173045 | 0.630657786 | 0.503799809 |
| 0.094875878 | 0.315289223 | 0.499068959 |
| 0.094867676 | 0.440784012 | 0.504251489 |
| 0.094229375 | 0.566361135 | 0.505734815 |
| 0.098065233 | 0.691859138 | 0.499854122 |
| 0.157370025 | 0.252402228 | 0.496213858 |
| 0.157360032 | 0.378020889 | 0.502708685 |
| 0.157285243 | 0.503724632 | 0.506639249 |
| 0.157215296 | 0.627605344 | 0.503724450 |
| 0.219870150 | 0.315287355 | 0.499890568 |
| 0.219793493 | 0.440809863 | 0.505742914 |
| 0.220283054 | 0.566289597 | 0.506898355 |
| 0.216047925 | 0.691793095 | 0.494498729 |
| 0.282346281 | 0.252387585 | 0.496325157 |
| 0.282354560 | 0.378052263 | 0.503136858 |
| 0.282354870 | 0.503419855 | 0.507201183 |
| 0.282279046 | 0.630282570 | 0.503663233 |
| 0.344845038 | 0.315284113 | 0.499572428 |
| 0.344895476 | 0.440806594 | 0.505123147 |
| 0.344428946 | 0.566339871 | 0.506492486 |
| 0.347658996 | 0.691485680 | 0.497445355 |
| 0.407327830 | 0.252383492 | 0.496006352 |
| 0.407345056 | 0.378021164 | 0.501738414 |
| 0.407383551 | 0.503716885 | 0.504756160 |
| 0.407399586 | 0.627826386 | 0.505419015 |
| 0.469833225 | 0.315280102 | 0.498174268 |
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| 0.470326521 | 0.566328718 | 0.501523252 |
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| 0.532322822 | 0.252383602 | 0.495406992 |
| 0.532325392 | 0.378035944 | 0.499041624 |
| 0.532335527 | 0.503419635 | 0.499257609 |
| 0.532411518 | 0.630191966 | 0.496642633 |
| 0.594831358 | 0.315277712 | 0.496477267 |
| 0.594841921 | 0.440785605 | 0.498000582 |
| 0.594370466 | 0.566280861 | 0.493638016 |
| 0.599267027 | 0.690615085 | 0.501277971 |
| 0.657343557 | 0.252390772 | 0.494873847 |
| 0.657317053 | 0.378011412 | 0.496797274 |
| 0.657315197 | 0.503686171 | 0.495015517 |
| 0.657465418 | 0.627681387 | 0.486511907 |
| 0.719853520 | 0.315285377 | 0.495580678 |

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| 0.719762207 | 0.440779287 | 0.496435379 |
| 0.720319693 | 0.566301410 | 0.492223943 |
| 0.716419337 | 0.692629680 | 0.501534451 |
| 0.782370096 | 0.252401541 | 0.494781594 |
| 0.782328033 | 0.378045422 | 0.496646777 |
| 0.782313805 | 0.503378207 | 0.496367297 |
| 0.782341832 | 0.630400645 | 0.494675705 |
| 0.844864404 | 0.315297162 | 0.496095663 |
| 0.844874777 | 0.440778545 | 0.498240959 |
| 0.844312723 | 0.566246686 | 0.498209132 |
| 0.848666121 | 0.690739644 | 0.498432267 |
| 0.907384122 | 0.252398986 | 0.495178225 |
| 0.907345960 | 0.378015065 | 0.498459285 |
| 0.907315506 | 0.503683534 | 0.500584649 |
| 0.907284006 | 0.627489137 | 0.503486383 |
| 0.969873481 | 0.315294031 | 0.497562285 |
| 0.969784024 | 0.440773517 | 0.501422109 |
| 0.970302968 | 0.566303498 | 0.503367238 |
| 0.966054920 | 0.692807590 | 0.499080823 |
| 0.032381757 | 0.294313146 | 0.497495404 |
| 0.032335072 | 0.419864583 | 0.502395575 |
| 0.032278246 | 0.545160418 | 0.504702092 |
| 0.032015410 | 0.674213275 | 0.501176069 |
| 0.094862989 | 0.357079675 | 0.501056924 |
| 0.094887464 | 0.482625287 | 0.505386240 |
| 0.093698470 | 0.608245322 | 0.504911307 |
| 0.127238426 | 0.731360877 | 0.491013707 |
| 0.157377020 | 0.294309630 | 0.498528063 |
| 0.157349231 | 0.419837962 | 0.504577823 |
| 0.157274323 | 0.545664368 | 0.506887630 |
| 0.157376449 | 0.668256028 | 0.500159260 |
| 0.219875241 | 0.357082477 | 0.502182438 |
| 0.219759328 | 0.482662155 | 0.507035849 |
| 0.220788175 | 0.608163730 | 0.505178385 |
| 0.192984495 | 0.732737841 | 0.481557226 |
| 0.282360223 | 0.294295262 | 0.498770402 |
| 0.282353989 | 0.419892330 | 0.505106854 |
| 0.282406331 | 0.545219813 | 0.507458581 |
| 0.282280735 | 0.673818443 | 0.497844770 |
| 0.344843682 | 0.357084070 | 0.501756415 |
| 0.344972228 | 0.482664738 | 0.506348601 |
| 0.344044544 | 0.608273454 | 0.506150555 |
| 0.371452105 | 0.732378669 | 0.485814757 |
| 0.407332398 | 0.294298531 | 0.498020576 |
| 0.407352050 | 0.419850325 | 0.503376255 |
| 0.407440555 | 0.545684753 | 0.504973347 |

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| 0.407473007 | 0.668664650 | 0.504850849 |
| 0.469840458 | 0.357082917 | 0.499784331 |
| 0.469801059 | 0.482664738 | 0.502421549 |
| 0.470863927 | 0.608306036 | 0.501690927 |
| 0.442493185 | 0.732107243 | 0.479627124 |
| 0.532329389 | 0.294299465 | 0.496632572 |
| 0.532315447 | 0.419882824 | 0.499807648 |
| 0.532350706 | 0.545260197 | 0.498074517 |
| 0.532674653 | 0.674098550 | 0.498513226 |
| 0.594810944 | 0.357081378 | 0.497363732 |
| 0.594879988 | 0.482656166 | 0.497198682 |
| 0.593924753 | 0.608265377 | 0.490890829 |
| 0.630372573 | 0.730827037 | 0.531495354 |
| 0.657343795 | 0.294308283 | 0.495451283 |
| 0.657291548 | 0.419838484 | 0.496891836 |
| 0.657293214 | 0.545647171 | 0.492582990 |
| 0.657380529 | 0.668590200 | 0.486372673 |
| 0.719831251 | 0.357086928 | 0.496126983 |
| 0.719714576 | 0.482629243 | 0.495566947 |
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| 0.695887564 | 0.731444558 | 0.528351187 |
| 0.782362340 | 0.294315042 | 0.495273136 |
| 0.782312711 | 0.419879940 | 0.496947264 |
| 0.782271218 | 0.545174209 | 0.495339890 |
| 0.782447514 | 0.674033716 | 0.497207161 |
| 0.844829954 | 0.357093988 | 0.496931857 |
| 0.844877823 | 0.482626112 | 0.498423598 |
| 0.843734776 | 0.608160268 | 0.498889957 |
| 0.879722132 | 0.732850587 | 0.487553741 |
| 0.907370322 | 0.294315783 | 0.496173458 |
| 0.907326260 | 0.419828704 | 0.499430378 |
| 0.907272777 | 0.545623105 | 0.501031457 |
| 0.907088724 | 0.668224490 | 0.504572381 |
| 0.969866248 | 0.357088081 | 0.499001382 |
| 0.969719216 | 0.482612815 | 0.502299652 |
| 0.970720749 | 0.608167411 | 0.504179831 |
| 0.945314495 | 0.733132947 | 0.488725982 |
| 0.094876746 | 0.233508355 | 0.495081290 |
| 0.219856541 | 0.233496817 | 0.495224036 |
| 0.344835735 | 0.233486735 | 0.495184078 |
| 0.469820520 | 0.233491625 | 0.494986063 |
| 0.594835164 | 0.233496954 | 0.494721958 |
| 0.719855090 | 0.233505910 | 0.494536535 |
| 0.844878108 | 0.233508163 | 0.494628883 |
| 0.969886519 | 0.233515416 | 0.494853663 |
| 0.844782180 | 0.762106442 | 0.476387256 |

| | | |
|---|---|---|
| 0.473073887 | 0.762351769 | 0.460732860 |
| 0.209842585 | 0.761346944 | 0.596178127 |
| 0.595783928 | 0.757562313 | 0.561568599 |
| 0.102353352 | 0.765832723 | 0.516186528 |
| 0.340440821 | 0.763433846 | 0.475287590 |
| 0.147354189 | 0.773451821 | 0.556157556 |
| 0.246617088 | 0.774336372 | 0.565438926 |

IM6
E+ZPE = -1210.33812 eV
1.0

| | | |
|---|---|---|
| 20.0422000885 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 34.7140998840 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 15.0721998215 |

  B   N   O   H
 64   64   14   2
Direct

| | | |
|---|---|---|
| 0.032369516 | 0.252458327 | 0.496116733 |
| 0.032347937 | 0.378101850 | 0.501137567 |
| 0.032337567 | 0.503433481 | 0.503222341 |
| 0.032208399 | 0.630573940 | 0.502724820 |
| 0.094865112 | 0.315347629 | 0.499644275 |
| 0.094903762 | 0.440845632 | 0.503539912 |
| 0.094293654 | 0.566348772 | 0.504199256 |
| 0.098494113 | 0.690940082 | 0.500953187 |
| 0.157374367 | 0.252461046 | 0.496602897 |
| 0.157362090 | 0.378081136 | 0.502656453 |
| 0.157357713 | 0.503771500 | 0.505058102 |
| 0.157318706 | 0.627562652 | 0.501980246 |
| 0.219878144 | 0.315352711 | 0.500277582 |
| 0.219826468 | 0.440869121 | 0.504552893 |
| 0.220352716 | 0.566366080 | 0.505566791 |
| 0.216093082 | 0.692811931 | 0.500283308 |
| 0.282363911 | 0.252464700 | 0.496720523 |
| 0.282370073 | 0.378120092 | 0.502749813 |
| 0.282406212 | 0.503510459 | 0.505439706 |
| 0.282267864 | 0.630550919 | 0.504996663 |
| 0.344873160 | 0.315358838 | 0.499867188 |
| 0.344926619 | 0.440877472 | 0.503638081 |
| 0.344427685 | 0.566506024 | 0.506200383 |
| 0.347831819 | 0.691654030 | 0.499869593 |
| 0.407353097 | 0.252463436 | 0.496457683 |
| 0.407369561 | 0.378098938 | 0.501216596 |
| 0.407366230 | 0.503825565 | 0.503189281 |
| 0.407434893 | 0.628006604 | 0.508471498 |

| | | |
|---|---|---|
| 0.469873671 | 0.315360870 | 0.498504873 |
| 0.469807007 | 0.440892445 | 0.500463195 |
| 0.470318908 | 0.566447837 | 0.501639074 |
| 0.466835096 | 0.691602163 | 0.498428091 |
| 0.532351896 | 0.252461486 | 0.495897015 |
| 0.532351610 | 0.378129158 | 0.498516294 |
| 0.532326677 | 0.503514964 | 0.497969704 |
| 0.532461956 | 0.630234493 | 0.498148579 |
| 0.594855958 | 0.315362739 | 0.496775887 |
| 0.594868901 | 0.440882170 | 0.496864059 |
| 0.594394923 | 0.566356959 | 0.493626880 |
| 0.599265599 | 0.690612118 | 0.502698372 |
| 0.657358070 | 0.252460057 | 0.495335650 |
| 0.657346079 | 0.378100092 | 0.496609097 |
| 0.657338180 | 0.503769632 | 0.494240983 |
| 0.657496204 | 0.627769244 | 0.487296754 |
| 0.719846477 | 0.315360761 | 0.495952126 |
| 0.719796895 | 0.440862885 | 0.496066462 |
| 0.720351289 | 0.566387673 | 0.492053895 |
| 0.716357811 | 0.692719129 | 0.503160903 |
| 0.782364529 | 0.252457502 | 0.495176865 |
| 0.782350254 | 0.378116246 | 0.496990891 |
| 0.782340166 | 0.503468371 | 0.495863765 |
| 0.782358105 | 0.630491578 | 0.495110807 |
| 0.844856315 | 0.315352354 | 0.496616279 |
| 0.844895524 | 0.440858132 | 0.498250766 |
| 0.844346507 | 0.566346959 | 0.497638055 |
| 0.848619299 | 0.690801567 | 0.499450531 |
| 0.907370703 | 0.252455827 | 0.495519081 |
| 0.907346055 | 0.378081795 | 0.498911375 |
| 0.907331875 | 0.503757159 | 0.500006675 |
| 0.907354430 | 0.627600729 | 0.502942039 |
| 0.969865487 | 0.315348096 | 0.498165726 |
| 0.969799822 | 0.440843846 | 0.501184896 |
| 0.970321716 | 0.566342948 | 0.502321070 |
| 0.965994394 | 0.693125334 | 0.499634816 |
| 0.032368722 | 0.294378008 | 0.498102452 |
| 0.032350867 | 0.419951505 | 0.502176806 |
| 0.032320158 | 0.545231131 | 0.503515900 |
| 0.032295150 | 0.674351680 | 0.501358614 |
| 0.094851515 | 0.357157092 | 0.501442957 |
| 0.094942845 | 0.482707759 | 0.504215707 |
| 0.093756528 | 0.608300487 | 0.503156663 |
| 0.130003160 | 0.733265253 | 0.504559347 |
| 0.157374189 | 0.294381524 | 0.499086232 |
| 0.157369870 | 0.419915022 | 0.503937651 |

| | | |
|---|---|---|
| 0.157328663 | 0.545737829 | 0.505175158 |
| 0.157140852 | 0.668304544 | 0.499245967 |
| 0.219880404 | 0.357163850 | 0.502229513 |
| 0.219810837 | 0.482741825 | 0.505320720 |
| 0.220806756 | 0.608253894 | 0.504405623 |
| 0.195454140 | 0.733368824 | 0.502870381 |
| 0.282377448 | 0.294383118 | 0.499194778 |
| 0.282380422 | 0.419974224 | 0.504040534 |
| 0.282436094 | 0.545329921 | 0.506119361 |
| 0.282190850 | 0.674143825 | 0.501512337 |
| 0.344864357 | 0.357171762 | 0.501624869 |
| 0.344981578 | 0.482750066 | 0.504483355 |
| 0.343971051 | 0.608469496 | 0.507607527 |
| 0.371807695 | 0.732176803 | 0.482542873 |
| 0.407371512 | 0.294389409 | 0.498476274 |
| 0.407377174 | 0.419939664 | 0.502090627 |
| 0.407389546 | 0.545809807 | 0.504309479 |
| 0.407535294 | 0.668835802 | 0.509567020 |
| 0.469871720 | 0.357176157 | 0.499638169 |
| 0.469776696 | 0.482773198 | 0.500663267 |
| 0.470846036 | 0.608410046 | 0.503389764 |
| 0.443131705 | 0.731652358 | 0.477504417 |
| 0.532363173 | 0.294389876 | 0.497126234 |
| 0.532335384 | 0.419989252 | 0.498572355 |
| 0.532333481 | 0.545359317 | 0.497520745 |
| 0.532793183 | 0.674052122 | 0.500180014 |
| 0.594844062 | 0.357179729 | 0.497238355 |
| 0.594890408 | 0.482756660 | 0.495931056 |
| 0.593973288 | 0.608330761 | 0.491681149 |
| 0.630155260 | 0.730753356 | 0.533389137 |
| 0.657350409 | 0.294389189 | 0.495878096 |
| 0.657326522 | 0.419936972 | 0.496247140 |
| 0.657339512 | 0.545733269 | 0.492235649 |
| 0.657459803 | 0.668661518 | 0.487543174 |
| 0.719849332 | 0.357175910 | 0.496356540 |
| 0.719754403 | 0.482724847 | 0.494995459 |
| 0.720825932 | 0.608303673 | 0.489927012 |
| 0.695725305 | 0.731422580 | 0.530582061 |
| 0.782352015 | 0.294387404 | 0.495714059 |
| 0.782346971 | 0.419967082 | 0.497074792 |
| 0.782335218 | 0.545276296 | 0.494805828 |
| 0.782500046 | 0.674128111 | 0.498399206 |
| 0.844841755 | 0.357165196 | 0.497483319 |
| 0.844904945 | 0.482722979 | 0.498097106 |
| 0.843835843 | 0.608279718 | 0.498585800 |
| 0.879459282 | 0.732996245 | 0.489334453 |

```
0.907362709        0.294382898        0.496696763
0.907345389        0.419913676        0.499596598
0.907309701        0.545717500        0.500241105
0.907293808        0.668350972        0.504551406
0.969855304        0.357158246        0.499549080
0.969745482        0.482700946        0.501691876
0.970781751        0.608236311        0.503085132
0.945104938        0.733415966        0.490280902
0.094870322        0.233587091        0.495336694
0.219873171        0.233587091        0.495545150
0.344858766        0.233586926        0.495584538
0.469852687        0.233585085        0.495440052
0.594855530        0.233582860        0.495183382
0.719858992        0.233578410        0.494974041
0.844864690        0.233573712        0.494931205
0.969868342        0.233579701        0.495083694
0.844415884        0.762203474        0.478746639
0.474047679        0.761247825        0.454417984
0.209868851        0.815277382        0.588471007
0.595371714        0.757405666        0.563410813
0.095745832        0.763170497        0.510416754
0.341016104        0.762678909        0.466064969
0.168030995        0.806224728        0.562529790
0.243018243        0.800258305        0.556071883
```

IM7 (13O)
E+ZPE = -1196.18745 eV
1.0
```
    20.0422000885         0.0000000000         0.0000000000
     0.0000000000        34.7140998840         0.0000000000
     0.0000000000         0.0000000000        15.0721998215
   B    N    O
  64   64   13
Direct
   0.034255377        0.254210534        0.485035130
   0.034232088        0.379864360        0.492440023
   0.034218777        0.505248133        0.499146342
   0.033978558        0.632247934        0.509294500
   0.096731008        0.317103682        0.489373493
   0.096755187        0.442612922        0.496658071
   0.096177383        0.568254028        0.502287314
   0.099628160        0.692961819        0.520698135
   0.159252837        0.254218501        0.485391994
   0.159211797        0.379815679        0.494139112
   0.159173861        0.505537306        0.500864730
```

| | | |
|---|---|---|
| 0.159176097 | 0.629759333 | 0.503498658 |
| 0.221739270 | 0.317082941 | 0.490426906 |
| 0.221634206 | 0.442565450 | 0.499291840 |
| 0.222081251 | 0.568097985 | 0.506071810 |
| 0.218582902 | 0.692967204 | 0.521194327 |
| 0.284243737 | 0.254205506 | 0.485823362 |
| 0.284196820 | 0.379807410 | 0.495801060 |
| 0.284141861 | 0.505123794 | 0.505601528 |
| 0.284226369 | 0.631727060 | 0.514841202 |
| 0.346730860 | 0.317062309 | 0.491008297 |
| 0.346707544 | 0.442498939 | 0.501790109 |
| 0.346180107 | 0.567840515 | 0.514405246 |
| 0.350985831 | 0.692111388 | 0.516838848 |
| 0.409235874 | 0.254188529 | 0.486008090 |
| 0.409197379 | 0.379753317 | 0.496209492 |
| 0.409174396 | 0.505286155 | 0.508908878 |
| 0.409255526 | 0.629079560 | 0.526125028 |
| 0.471742934 | 0.317049919 | 0.490592019 |
| 0.471643961 | 0.442456357 | 0.501588519 |
| 0.472135734 | 0.567821065 | 0.516063144 |
| 0.468080399 | 0.694269059 | 0.516248220 |
| 0.534244998 | 0.254174325 | 0.485782804 |
| 0.534213403 | 0.379776558 | 0.494756031 |
| 0.534176763 | 0.505012751 | 0.506842674 |
| 0.534105008 | 0.631927168 | 0.518423507 |
| 0.596738402 | 0.317059864 | 0.489265453 |
| 0.596742351 | 0.442486824 | 0.498835668 |
| 0.596134474 | 0.567879251 | 0.510504736 |
| 0.600378335 | 0.692243530 | 0.519351132 |
| 0.659241322 | 0.254174325 | 0.485322994 |
| 0.659221242 | 0.379768591 | 0.492520064 |
| 0.659164665 | 0.505363242 | 0.502816662 |
| 0.659131072 | 0.629162911 | 0.510254868 |
| 0.721751761 | 0.317069342 | 0.488102008 |
| 0.721660591 | 0.442521824 | 0.496172635 |
| 0.722110824 | 0.567943591 | 0.506460026 |
| 0.717782503 | 0.694549001 | 0.519339015 |
| 0.784246640 | 0.254182155 | 0.484965624 |
| 0.784232745 | 0.379826118 | 0.491300337 |
| 0.784174836 | 0.505112420 | 0.500336110 |
| 0.783978412 | 0.632130408 | 0.511930831 |
| 0.846744135 | 0.317091347 | 0.487876658 |
| 0.846767832 | 0.442574076 | 0.495089800 |
| 0.846089104 | 0.568007327 | 0.505681158 |
| 0.850283478 | 0.692438638 | 0.517564345 |
| 0.909253289 | 0.254198226 | 0.484881027 |

| | | |
|---|---|---|
| 0.909242821 | 0.379833920 | 0.491405244 |
| 0.909186958 | 0.505488680 | 0.499452397 |
| 0.909092553 | 0.629161372 | 0.514112130 |
| 0.971743124 | 0.317102144 | 0.488418250 |
| 0.971690402 | 0.442615037 | 0.495332265 |
| 0.972130928 | 0.568070843 | 0.504252849 |
| 0.967719194 | 0.694549550 | 0.517648341 |
| 0.034242952 | 0.296124281 | 0.487622393 |
| 0.034231490 | 0.421701075 | 0.494697788 |
| 0.034214961 | 0.547044629 | 0.501457574 |
| 0.033911858 | 0.675718589 | 0.516312790 |
| 0.096715585 | 0.358897513 | 0.491991887 |
| 0.096791647 | 0.484470049 | 0.498577733 |
| 0.095695126 | 0.610206346 | 0.503770355 |
| 0.123771054 | 0.732473119 | 0.547799855 |
| 0.159236243 | 0.296122468 | 0.488431379 |
| 0.159199699 | 0.421638548 | 0.496689898 |
| 0.159154863 | 0.547508251 | 0.502259916 |
| 0.159278604 | 0.670587048 | 0.505865285 |
| 0.221715431 | 0.358871909 | 0.493589359 |
| 0.221582507 | 0.484424939 | 0.501834748 |
| 0.222606809 | 0.610046623 | 0.507078306 |
| 0.195212559 | 0.732036310 | 0.549940595 |
| 0.284235933 | 0.296100188 | 0.489167221 |
| 0.284173433 | 0.421632669 | 0.499157953 |
| 0.284104817 | 0.546934520 | 0.508850223 |
| 0.284583030 | 0.675485954 | 0.517322006 |
| 0.346691342 | 0.358845316 | 0.494499836 |
| 0.346712659 | 0.484324061 | 0.505883698 |
| 0.345743458 | 0.609737780 | 0.519766144 |
| 0.381736191 | 0.732816467 | 0.490246639 |
| 0.409234446 | 0.296085628 | 0.489296679 |
| 0.409166926 | 0.421547230 | 0.500111995 |
| 0.409131809 | 0.547185782 | 0.514255350 |
| 0.409253765 | 0.669939417 | 0.529779085 |
| 0.471712100 | 0.358832954 | 0.493952835 |
| 0.471594997 | 0.484260216 | 0.506163368 |
| 0.472587871 | 0.609663550 | 0.521778533 |
| 0.447321131 | 0.733461625 | 0.492677331 |
| 0.534243047 | 0.296080298 | 0.488530276 |
| 0.534190039 | 0.421588384 | 0.498407558 |
| 0.534128942 | 0.546766830 | 0.511466497 |
| 0.534225869 | 0.675584744 | 0.518976456 |
| 0.596710851 | 0.358844410 | 0.492012609 |
| 0.596740971 | 0.484306094 | 0.502714633 |
| 0.595598496 | 0.609792779 | 0.513031130 |

| | | |
|---|---|---|
| 0.631194527 | 0.734156728 | 0.534119695 |
| 0.659244320 | 0.296091287 | 0.487389166 |
| 0.659195832 | 0.421572258 | 0.495522846 |
| 0.659100238 | 0.547288693 | 0.506331992 |
| 0.659032955 | 0.669913373 | 0.511743415 |
| 0.721738675 | 0.358862486 | 0.490342309 |
| 0.721591595 | 0.484348127 | 0.499464356 |
| 0.722548496 | 0.609803054 | 0.509131254 |
| 0.696805970 | 0.734604251 | 0.533284861 |
| 0.784249209 | 0.296099913 | 0.486779397 |
| 0.784224942 | 0.421653493 | 0.493875925 |
| 0.784125873 | 0.546870455 | 0.503891872 |
| 0.784024854 | 0.675817544 | 0.516114174 |
| 0.846741661 | 0.358891579 | 0.489980415 |
| 0.846783439 | 0.484404830 | 0.498024689 |
| 0.845536756 | 0.609880855 | 0.510684244 |
| 0.881411055 | 0.734758974 | 0.511777772 |
| 0.909249578 | 0.296114968 | 0.486985764 |
| 0.909242631 | 0.421651955 | 0.493751498 |
| 0.909122911 | 0.547409351 | 0.503043530 |
| 0.908891180 | 0.669815297 | 0.520255440 |
| 0.971751023 | 0.358904189 | 0.490652730 |
| 0.971649480 | 0.484464005 | 0.497767165 |
| 0.972564793 | 0.609888657 | 0.509186270 |
| 0.947062040 | 0.734984522 | 0.512074653 |
| 0.096764519 | 0.235329903 | 0.483885415 |
| 0.221747692 | 0.235335672 | 0.484152430 |
| 0.346732882 | 0.235316002 | 0.484465983 |
| 0.471732656 | 0.235304244 | 0.484575351 |
| 0.596740591 | 0.235282293 | 0.484512426 |
| 0.721748097 | 0.235289436 | 0.484295681 |
| 0.846756793 | 0.235299958 | 0.484032558 |
| 0.971759874 | 0.235313722 | 0.483842895 |
| 0.846587015 | 0.764271255 | 0.505079204 |
| 0.346761575 | 0.760029101 | 0.463372008 |
| 0.226483065 | 0.760560029 | 0.579034490 |
| 0.596085321 | 0.763087366 | 0.548114895 |
| 0.092939362 | 0.761597381 | 0.573850157 |

IM8
E+ZPE = -1250.48040 eV
1.0

| | | |
|---|---|---|
| 20.0422000885 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 34.7140998840 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 15.0721998215 |

```
  B   N   O   H   C
 64  64  13   8   3
Direct
   0.021215094        0.249712860        0.504786373
   0.021188068        0.375377208        0.500810631
   0.021173857        0.500779333        0.494742206
   0.020945151        0.627842320        0.490050649
   0.083705207        0.312614140        0.503509224
   0.083704779        0.438145632        0.498544356
   0.083176984        0.563767810        0.490561015
   0.086549059        0.688757851        0.493393273
   0.146190480        0.249702036        0.505093219
   0.146177026        0.375370175        0.502264029
   0.146124208        0.501083176        0.495774232
   0.146138995        0.625230149        0.484155562
   0.208687904        0.312610239        0.504414007
   0.208599947        0.438156841        0.500712747
   0.209068404        0.563692811        0.493696007
   0.205517214        0.688765488        0.493853938
   0.271172125        0.249676981        0.505265545
   0.271164535        0.375381109        0.503591480
   0.271101225        0.500776695        0.500022652
   0.271203458        0.627436884        0.494711044
   0.333663554        0.312582932        0.504630878
   0.333664053        0.438128050        0.502924449
   0.333165547        0.563604515        0.501488799
   0.337886335        0.687776982        0.489048013
   0.396155839        0.249652833        0.505244854
   0.396156815        0.375323170        0.503555003
   0.396126456        0.501002023        0.503114333
   0.396240085        0.625035975        0.505592227
   0.458655238        0.312554855        0.503903262
   0.458587385        0.438080166        0.502586598
   0.459109374        0.563623910        0.502981237
   0.454982615        0.689897840        0.487585567
   0.521165201        0.249634839        0.504867964
   0.521156589        0.375316576        0.501999134
   0.521128705        0.500679553        0.501287272
   0.521067988        0.627707431        0.497428302
   0.583656749        0.312531119        0.502542212
   0.583680351        0.438055578        0.500226077
   0.583102213        0.563547153        0.497855590
   0.587311814        0.687961541        0.490503024
   0.646193073        0.249639344        0.504368070
   0.646156957        0.375283610        0.500230664
   0.646121936        0.500955650        0.497816012
```

| | | |
|---|---|---|
| 0.646090436 | 0.624751472 | 0.490024453 |
| 0.708681052 | 0.312546943 | 0.501686498 |
| 0.708608583 | 0.438057666 | 0.498100712 |
| 0.709096693 | 0.563535944 | 0.494458139 |
| 0.704708417 | 0.690270363 | 0.490339462 |
| 0.771213712 | 0.249657256 | 0.504280025 |
| 0.771170126 | 0.375316989 | 0.499405638 |
| 0.771149618 | 0.500655213 | 0.495882937 |
| 0.770930401 | 0.627766332 | 0.491997518 |
| 0.833695649 | 0.312569690 | 0.501784667 |
| 0.833712683 | 0.438071320 | 0.497306690 |
| 0.833085916 | 0.563597921 | 0.494337223 |
| 0.837197685 | 0.688106155 | 0.489424112 |
| 0.896221552 | 0.249691294 | 0.504477724 |
| 0.896196333 | 0.375325560 | 0.499739597 |
| 0.896141326 | 0.501020209 | 0.495299806 |
| 0.896057294 | 0.624892899 | 0.495539771 |
| 0.958712909 | 0.312599827 | 0.502492321 |
| 0.958639155 | 0.438128984 | 0.497579558 |
| 0.959120127 | 0.563641273 | 0.493106707 |
| 0.954640539 | 0.690234429 | 0.489738741 |
| 0.021215284 | 0.291628640 | 0.503607046 |
| 0.021181991 | 0.417223621 | 0.498969524 |
| 0.021203979 | 0.542580169 | 0.492545690 |
| 0.020835843 | 0.671426984 | 0.491255507 |
| 0.083686328 | 0.354427229 | 0.502325310 |
| 0.083740085 | 0.480001358 | 0.496101516 |
| 0.082672191 | 0.605705843 | 0.487058940 |
| 0.110681598 | 0.728882991 | 0.515267603 |
| 0.146196951 | 0.291628640 | 0.504453553 |
| 0.146159872 | 0.417201588 | 0.500499673 |
| 0.146141421 | 0.543040934 | 0.492543349 |
| 0.146212713 | 0.666060171 | 0.481507904 |
| 0.208679149 | 0.354428081 | 0.503693161 |
| 0.208541943 | 0.480025534 | 0.498745472 |
| 0.209573501 | 0.605618646 | 0.489871521 |
| 0.182116941 | 0.728473819 | 0.517648879 |
| 0.271171482 | 0.291605921 | 0.504905771 |
| 0.271130108 | 0.417235736 | 0.502667557 |
| 0.271084857 | 0.542607861 | 0.498550462 |
| 0.271501687 | 0.671204679 | 0.491949841 |
| 0.333651610 | 0.354401653 | 0.504132977 |
| 0.333665290 | 0.479998336 | 0.502510860 |
| 0.332733895 | 0.605572053 | 0.501866891 |
| 0.368546287 | 0.727825419 | 0.457544212 |
| 0.396155482 | 0.291583394 | 0.504754736 |

| | | |
|---|---|---|
| 0.396116488 | 0.417159583 | 0.503305736 |
| 0.396103712 | 0.542969781 | 0.503661524 |
| 0.396191598 | 0.665912975 | 0.504228109 |
| 0.458658998 | 0.354370692 | 0.503157929 |
| 0.458543560 | 0.479940150 | 0.502724757 |
| 0.459559036 | 0.605545899 | 0.503470311 |
| 0.434139982 | 0.728503104 | 0.459488994 |
| 0.521152211 | 0.291558257 | 0.503804744 |
| 0.521130323 | 0.417162495 | 0.501607184 |
| 0.521089449 | 0.542486104 | 0.501106784 |
| 0.521164202 | 0.671319238 | 0.492409050 |
| 0.583646233 | 0.354346901 | 0.501368706 |
| 0.583695434 | 0.479911909 | 0.499755605 |
| 0.582559430 | 0.605466340 | 0.495069047 |
| 0.618127768 | 0.730192428 | 0.499388270 |
| 0.646176038 | 0.291559713 | 0.502659490 |
| 0.646144633 | 0.417111616 | 0.499356854 |
| 0.646080253 | 0.542901045 | 0.496559269 |
| 0.645972810 | 0.665475067 | 0.485972214 |
| 0.708671250 | 0.354353412 | 0.500200040 |
| 0.708557621 | 0.479905535 | 0.497060840 |
| 0.709513903 | 0.605402055 | 0.491817473 |
| 0.683753248 | 0.730623412 | 0.498632307 |
| 0.771193632 | 0.291575949 | 0.502429490 |
| 0.771162751 | 0.417157110 | 0.498058920 |
| 0.771123827 | 0.542442808 | 0.494764478 |
| 0.770954478 | 0.671488357 | 0.490017082 |
| 0.833682991 | 0.354376159 | 0.500185550 |
| 0.833744088 | 0.479921854 | 0.495991578 |
| 0.832511110 | 0.605539361 | 0.494205170 |
| 0.868337729 | 0.730105396 | 0.476276717 |
| 0.896212511 | 0.291612157 | 0.502840231 |
| 0.896195666 | 0.417151891 | 0.498113842 |
| 0.896119533 | 0.542975055 | 0.494389297 |
| 0.895811764 | 0.665647208 | 0.496344423 |
| 0.958708627 | 0.354404482 | 0.501017220 |
| 0.958599566 | 0.479988117 | 0.495777269 |
| 0.959532104 | 0.605523097 | 0.493065104 |
| 0.933981196 | 0.730389459 | 0.477107881 |
| 0.083702405 | 0.230813932 | 0.505344036 |
| 0.208672154 | 0.230799619 | 0.505389498 |
| 0.333655345 | 0.230770251 | 0.505447868 |
| 0.458651289 | 0.230754427 | 0.505447932 |
| 0.583682254 | 0.230747697 | 0.505233054 |
| 0.708706747 | 0.230758356 | 0.505104893 |
| 0.833730670 | 0.230785306 | 0.505162472 |

```
    0.958728993        0.230816680        0.505278769
    0.833566983        0.759262735        0.463466570
    0.333489803        0.754433938        0.427799674
    0.213385448        0.757644785        0.543057173
    0.583008569        0.759443063        0.509106640
    0.079881311        0.758647631        0.537294201
    0.935058863        0.812873835        0.559925760
    0.818841660        0.838467860        0.546751093
    0.840992550        0.879889524        0.610036403
    0.876299179        0.872517841        0.503292449
    0.018858249        0.844793784        0.658724210
    0.996798785        0.876312693        0.570793909
    0.962827058        0.883709815        0.678296547
    0.900701806        0.820543427        0.666132742
    0.918354169        0.835580801        0.605981063
    0.860344589        0.857730630        0.564407248
    0.977411820        0.861412955        0.629964528
```

TS8
E+ZPE = -1249.47823 eV
1.0
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    20.0422000885         0.0000000000         0.0000000000
     0.0000000000        34.7140998840         0.0000000000
     0.0000000000         0.0000000000        15.0721998215
```
   B   N   O   H   C
  64  64  13   8   3
Direct
```
    0.015175214        0.253481668        0.508220681
    0.015212671        0.379167554        0.505851270
    0.015198673        0.504527976        0.498428502
    0.015124603        0.631349811        0.484662796
    0.077688237        0.316398058        0.508178351
    0.077754646        0.441934495        0.504871476
    0.077267940        0.567375136        0.493354581
    0.080877057        0.692012653        0.475670839
    0.140165707        0.253497931        0.508904038
    0.140209269        0.379160246        0.508642970
    0.140220998        0.504826654        0.502479318
    0.140434731        0.628484017        0.483282542
    0.202712130        0.316408442        0.509837863
    0.202671185        0.441951472        0.508531450
    0.203253414        0.567330740        0.497725910
    0.199895983        0.692311166        0.475724242
    0.265175699        0.253498783        0.509406336
    0.265215598        0.379187059        0.510859481
```

| | | |
|---|---|---|
| 0.265240841 | 0.504556052 | 0.506774117 |
| 0.265449470 | 0.631110418 | 0.489606752 |
| 0.327703529 | 0.316409184 | 0.510656182 |
| 0.327768266 | 0.441952159 | 0.510573452 |
| 0.327339612 | 0.567438102 | 0.503048971 |
| 0.332382016 | 0.691010411 | 0.471398755 |
| 0.390183419 | 0.253499854 | 0.509459391 |
| 0.390234429 | 0.379159367 | 0.510994064 |
| 0.390255151 | 0.504857862 | 0.507798139 |
| 0.390496874 | 0.628900221 | 0.498849810 |
| 0.452719934 | 0.316401052 | 0.510073020 |
| 0.452693192 | 0.441929714 | 0.508873698 |
| 0.453251201 | 0.567432608 | 0.501481048 |
| 0.449403805 | 0.692989731 | 0.471098426 |
| 0.515194399 | 0.253497217 | 0.508992020 |
| 0.515236320 | 0.379167196 | 0.508715324 |
| 0.515216335 | 0.504498306 | 0.503092219 |
| 0.515238033 | 0.631271186 | 0.488336848 |
| 0.577709787 | 0.316398470 | 0.508381555 |
| 0.577760939 | 0.441901143 | 0.504337920 |
| 0.577188321 | 0.567235247 | 0.492918910 |
| 0.581385027 | 0.691363923 | 0.475981893 |
| 0.640181540 | 0.253487354 | 0.508268833 |
| 0.640219940 | 0.379131730 | 0.505598776 |
| 0.640190771 | 0.504737479 | 0.496753393 |
| 0.640147946 | 0.628259623 | 0.478717090 |
| 0.702708300 | 0.316385448 | 0.506696354 |
| 0.702678132 | 0.441878918 | 0.500439594 |
| 0.703173331 | 0.567252500 | 0.487253507 |
| 0.698671474 | 0.693733295 | 0.476387667 |
| 0.765175628 | 0.253473811 | 0.507755271 |
| 0.765208698 | 0.379149175 | 0.503704076 |
| 0.765210792 | 0.504471328 | 0.493815562 |
| 0.764944896 | 0.631586952 | 0.479825899 |
| 0.827689778 | 0.316383030 | 0.506019103 |
| 0.827775618 | 0.441896391 | 0.499439205 |
| 0.827173023 | 0.567468321 | 0.487444277 |
| 0.830742343 | 0.692592757 | 0.478367977 |
| 0.890170667 | 0.253471228 | 0.507747837 |
| 0.890209590 | 0.379132939 | 0.503865297 |
| 0.890172095 | 0.504831159 | 0.494890963 |
| 0.890232050 | 0.628855277 | 0.484004780 |
| 0.952690004 | 0.316384486 | 0.506632099 |
| 0.952676871 | 0.441924769 | 0.501403823 |
| 0.953166218 | 0.567387059 | 0.490419345 |
| 0.948982978 | 0.693673955 | 0.479701028 |

| | | |
|---|---|---|
| 0.015195730 | 0.295391047 | 0.507656153 |
| 0.015223767 | 0.421005917 | 0.504215897 |
| 0.015243655 | 0.546286725 | 0.494405938 |
| 0.015249618 | 0.674954696 | 0.480637416 |
| 0.077709905 | 0.358199059 | 0.507697091 |
| 0.077792367 | 0.483772419 | 0.502243686 |
| 0.076886619 | 0.609213444 | 0.487142525 |
| 0.104543719 | 0.732977894 | 0.474947557 |
| 0.140199681 | 0.295413931 | 0.509056875 |
| 0.140216573 | 0.420988115 | 0.507731069 |
| 0.140264014 | 0.546737599 | 0.498049429 |
| 0.140701804 | 0.669066019 | 0.474175111 |
| 0.202719339 | 0.358213070 | 0.510111617 |
| 0.202647869 | 0.483802638 | 0.506481698 |
| 0.203854938 | 0.609146082 | 0.490360374 |
| 0.175495164 | 0.733370802 | 0.481278252 |
| 0.265200347 | 0.295411844 | 0.510138287 |
| 0.265212814 | 0.421033802 | 0.510644603 |
| 0.265272174 | 0.546355955 | 0.503374103 |
| 0.265784194 | 0.674716291 | 0.477882288 |
| 0.327712808 | 0.358213427 | 0.511283573 |
| 0.327803526 | 0.483813352 | 0.509381818 |
| 0.326937057 | 0.609392893 | 0.498817889 |
| 0.363425846 | 0.729605236 | 0.431991686 |
| 0.390201810 | 0.295414783 | 0.510289922 |
| 0.390225983 | 0.420984928 | 0.510851192 |
| 0.390246658 | 0.546807599 | 0.505566538 |
| 0.390392619 | 0.669681013 | 0.491513506 |
| 0.452732924 | 0.358203015 | 0.510326558 |
| 0.452645371 | 0.483772089 | 0.507436150 |
| 0.453706526 | 0.609303224 | 0.498118303 |
| 0.428944264 | 0.730420612 | 0.435333836 |
| 0.515211957 | 0.295404728 | 0.509327529 |
| 0.515222473 | 0.420998829 | 0.507682317 |
| 0.515181980 | 0.546249582 | 0.499700083 |
| 0.515272198 | 0.674624919 | 0.479094106 |
| 0.577718018 | 0.358189719 | 0.507757897 |
| 0.577763936 | 0.483714232 | 0.501549890 |
| 0.576639781 | 0.609009435 | 0.486456954 |
| 0.611585776 | 0.733459702 | 0.484194665 |
| 0.640199669 | 0.295398245 | 0.507818513 |
| 0.640212897 | 0.420932978 | 0.503465882 |
| 0.640152466 | 0.546591007 | 0.491920039 |
| 0.639919641 | 0.668855527 | 0.471996534 |
| 0.702715770 | 0.358174829 | 0.505375515 |
| 0.702629882 | 0.483678628 | 0.496755260 |

| | | |
|---|---|---|
| 0.703600106 | 0.608975699 | 0.481093113 |
| 0.677188273 | 0.734088762 | 0.483765701 |
| 0.765193900 | 0.295383712 | 0.506746815 |
| 0.765231443 | 0.420960945 | 0.501087359 |
| 0.765238628 | 0.546188209 | 0.489155927 |
| 0.764631798 | 0.675044255 | 0.476908315 |
| 0.827703196 | 0.358174664 | 0.504525053 |
| 0.827798553 | 0.483704672 | 0.495800206 |
| 0.826691289 | 0.609345476 | 0.483309307 |
| 0.856743959 | 0.732970861 | 0.470859093 |
| 0.890185418 | 0.295383437 | 0.506712742 |
| 0.890236713 | 0.420938143 | 0.501531667 |
| 0.890176758 | 0.546735731 | 0.490780385 |
| 0.890345869 | 0.669553817 | 0.481858504 |
| 0.952718078 | 0.358184361 | 0.505460396 |
| 0.952619105 | 0.483756100 | 0.498365798 |
| 0.953689444 | 0.609224104 | 0.486485427 |
| 0.925713690 | 0.733888873 | 0.471843158 |
| 0.077674367 | 0.234574663 | 0.508650911 |
| 0.202672850 | 0.234588399 | 0.508991672 |
| 0.327675217 | 0.234595624 | 0.509129514 |
| 0.452685816 | 0.234596421 | 0.508989109 |
| 0.577677430 | 0.234577493 | 0.508633321 |
| 0.702672136 | 0.234563152 | 0.508262347 |
| 0.827677406 | 0.234559581 | 0.508141811 |
| 0.952681344 | 0.234574443 | 0.508283987 |
| 0.825055756 | 0.764204333 | 0.461329785 |
| 0.205525636 | 0.764589659 | 0.491928740 |
| 0.576060168 | 0.762695557 | 0.493603880 |
| 0.328897752 | 0.754796956 | 0.395222909 |
| 0.072622910 | 0.764129663 | 0.476402283 |
| 0.943329414 | 0.759528117 | 0.517096942 |
| 0.892516144 | 0.787222010 | 0.610151688 |
| 0.982020835 | 0.749608108 | 0.688996515 |
| 0.045396133 | 0.778092433 | 0.636283929 |
| 0.992101646 | 0.798617662 | 0.717642811 |
| 0.925723778 | 0.827341874 | 0.479252860 |
| 0.952486252 | 0.851575418 | 0.576324223 |
| 0.011649403 | 0.825356235 | 0.512262829 |
| 0.945147002 | 0.790337637 | 0.591286752 |
| 0.993822068 | 0.778131169 | 0.661078310 |
| 0.959849960 | 0.825067117 | 0.536185772 |

TS8#
E+ZPE = -1241.50 eV

```
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  20.0422000000000011   0.0000000000000000   0.0000000000000000
   0.0000000000000000  34.7141000000000020   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.0722000000000005
  B   N   O   H   C
  64   64   13   6   3
Direct
 0.7799120180037671 0.2535815325661765 0.5049890516313353
 0.7798967392829331 0.3792840369632169 0.5043126178528149
 0.7798853151432509 0.5047026562033764 0.4998774389123203
 0.7798678229039055 0.6315786401956226 0.4910238985935757
 0.8424046564461767 0.3164890123615592 0.5055010121924660
 0.8424080485722406 0.4420224419602500 0.5037137024516973
 0.8419807402367545 0.5675382355824373 0.4954395065421768
 0.8456491656273173 0.6922111913746584 0.4889852139053838
 0.9048957468199407 0.2535595344423696 0.5053539824702519
 0.9048914340913978 0.3792214518174387 0.5061797614608363
 0.9048719781868034 0.5048890054099247 0.5019645007244833
 0.9051656712539564 0.6287253427715913 0.4871241452968201
 0.9674060542294231 0.3164546625958981 0.5067271054492356
 0.9673304236166262 0.4419759044340642 0.5063944224883073
 0.9679012612943464 0.5673889376497185 0.4993899631555623
 0.9644286941007637 0.6924775933291719 0.4920781824544512
 0.0298959325213514 0.2535380992302971 0.5057396423294850
 0.0298783272084495 0.3792100501331444 0.5079520853971150
 0.0298678557994935 0.5045509199292368 0.5062563039317594
 0.0300455433480080 0.6311807545125725 0.4978790517947730
 0.0923954971245852 0.3164334212060079 0.5074718151342130
 0.0924147173677345 0.4419416252585989 0.5086889928376856
 0.0919483331142196 0.5673978629597858 0.5066408791092414
 0.0967793350915496 0.6914670536400433 0.4890691797840518
 0.1549100120163498 0.2535320254537992 0.5058465884931863
 0.1548878901354798 0.3791630969568504 0.5085077040268058
 0.1548726449771372 0.5048218222323284 0.5088678638312010
 0.1550210026484070 0.6288565498100793 0.5085435286853481
 0.2174325345246823 0.3164249417070333 0.5070885649971405
 0.2173417051777675 0.4419277445100853 0.5084426828040435
 0.2178505686633660 0.5674419016932047 0.5072685343804834
 0.2137737722793761 0.6935321669007340 0.4877209252174541
 0.2799522939218743 0.2535399493984872 0.5055810536844018
 0.2799118826461063 0.3792029420973904 0.5071050251914864
 0.2798536645327849 0.5045347542983690 0.5064082424998710
 0.2797422484939111 0.6314800986135103 0.4992789329722036
 0.3424482299128861 0.3164575770769228 0.5058412417227993
 0.3424349893138894 0.4419599111881657 0.5054720933209751
 0.3417980125895389 0.5673821858570510 0.5009154836063953
```

0.3458908135500957 0.6917163976172721 0.4900719579634342
0.4049763995985729 0.2535615572886560 0.5052024008297827
0.4049271754253795 0.3792136311436693 0.5047369689534340
0.4048502230073028 0.5048728353591130 0.5019667633328342
0.4046600336193427 0.6285244074905756 0.4904834491419333
0.4674528310943104 0.3164855031741217 0.5045747594649980
0.4673765798992192 0.4420189896155143 0.5024751371246958
0.4678012596273859 0.5674838704573628 0.4968894277978250
0.4631921439151252 0.6939025248118543 0.4889429245176521
0.5299742924223817 0.2535774721885364 0.5049021888563858
0.5299244732401542 0.3792792031730406 0.5030626891037623
0.5299123601767264 0.5046945285110445 0.4997737144113537
0.5294886016221714 0.6318382989714451 0.4921230638927340
0.5924393273572269 0.3165067981136837 0.5040319401288402
0.5924630352717307 0.4420667848607497 0.5013742611925722
0.5918642944772387 0.5677703661334642 0.4970415044977630
0.5951025003399021 0.6928038360531025 0.4868294122947490
0.6549394440530334 0.2535867808872004 0.5048110095708698
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0.6548722931280107 0.5050502762800048 0.4994655960742173
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0.0923981639918550 0.2346330069842417 0.5052923180924681

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0.2174257339596600  0.2346371822248767  0.5053182835988214
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0.4674840579800011  0.2346546061178830  0.5051230315969261
0.5924646175797791  0.2346639154603745  0.5050051490737376
0.7174245746320083  0.2346671035409189  0.5049541932932707
0.5915164538718071  0.7633471749779084  0.4477820915853027
0.9702942096643332  0.7627612196910851  0.5328356754218508
0.3412020134518821  0.7630725049816988  0.5089072863481209
0.0922460249544882  0.7574696078174245  0.4243947242368556
0.8368930684986015  0.7630811648450495  0.5194985422917222
0.7052634376000709  0.7632084626481749  0.4844341390340391
0.7619480118483510  0.7960986391524992  0.6323124886404494
0.7256796581662919  0.8433233898819595  0.6257972808392479
0.6754868055767493  0.8030658955173265  0.6551590341105601
0.6768884277987861  0.8162872165644796  0.3840188055458920
0.7137950612159270  0.8578293466093173  0.4458029073112404
0.7014811826855226  0.8062725552749671  0.5182737500840465
0.7171946728315272  0.8123227092807390  0.6124843370368467
0.6966988882035018  0.8276637922288322  0.4465089967937185
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IM9
E+ZPE = -1251.77398 eV
1.0
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    20.0422000885      0.0000000000      0.0000000000
     0.0000000000     34.7140998840      0.0000000000
     0.0000000000      0.0000000000     15.0721998215
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  B   N   O   H   C
 64  64  13   8   3
Direct
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   0.022772432      0.251754433      0.501042245
   0.022681264      0.377446225      0.503041632
   0.022593999      0.502843982      0.500163309
   0.022737561      0.629534171      0.492024346
   0.085204141      0.314658790      0.503295707
   0.085186386      0.440180007      0.504048475
   0.084752248      0.565574660      0.497006899
   0.088206797      0.689980641      0.490330603
   0.147751296      0.251760367      0.501647964
   0.147666657      0.377376638      0.505684797
   0.147653988      0.502992991      0.503774816
   0.147982824      0.626748320      0.490931166
   0.210218588      0.314632334      0.504655365
   0.210124397      0.440098552      0.507464402
   0.210680622      0.565501693      0.502627853
   0.206896987      0.690845742      0.493921894
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| | | |
|---|---|---|
| 0.272757077 | 0.251739021 | 0.502077814 |
| 0.272719225 | 0.377348396 | 0.507289640 |
| 0.272642544 | 0.502681566 | 0.508678245 |
| 0.272757957 | 0.629439556 | 0.501335677 |
| 0.335242915 | 0.314597499 | 0.504891344 |
| 0.335227998 | 0.440074788 | 0.509162068 |
| 0.334688403 | 0.565589165 | 0.509884432 |
| 0.339530553 | 0.689654875 | 0.490548328 |
| 0.397778097 | 0.251715285 | 0.502042160 |
| 0.397743813 | 0.377316693 | 0.506665097 |
| 0.397661042 | 0.502972827 | 0.510326969 |
| 0.397783260 | 0.627077602 | 0.511419959 |
| 0.460271644 | 0.314599587 | 0.503674274 |
| 0.460160441 | 0.440072728 | 0.507255124 |
| 0.460595210 | 0.565597901 | 0.509332432 |
| 0.456563048 | 0.691639250 | 0.489227268 |
| 0.522788839 | 0.251694763 | 0.501493703 |
| 0.522762050 | 0.377357709 | 0.503914651 |
| 0.522650562 | 0.502670357 | 0.506174694 |
| 0.522506337 | 0.629611423 | 0.501381993 |
| 0.585261830 | 0.314599807 | 0.501631545 |
| 0.585247317 | 0.440100887 | 0.502985191 |
| 0.584536898 | 0.565498726 | 0.501613195 |
| 0.588687495 | 0.689833994 | 0.492151147 |
| 0.647780024 | 0.251706713 | 0.500834454 |
| 0.647751522 | 0.377355045 | 0.500927561 |
| 0.647639653 | 0.503015793 | 0.500719612 |
| 0.647376137 | 0.626613816 | 0.491879070 |
| 0.710269146 | 0.314615493 | 0.500227817 |
| 0.710174835 | 0.440169732 | 0.499915909 |
| 0.710550030 | 0.565660043 | 0.496490839 |
| 0.706246309 | 0.691707876 | 0.490976818 |
| 0.772793003 | 0.251720614 | 0.500435292 |
| 0.772737330 | 0.377410978 | 0.499808629 |
| 0.772672093 | 0.502855300 | 0.498353523 |
| 0.772246175 | 0.630176032 | 0.492408671 |
| 0.835252479 | 0.314641510 | 0.500256670 |
| 0.835231923 | 0.440210776 | 0.499509470 |
| 0.834537968 | 0.565981963 | 0.496126730 |
| 0.838169146 | 0.691834413 | 0.490702495 |
| 0.897788851 | 0.251744598 | 0.500530487 |
| 0.897714240 | 0.377415484 | 0.500731413 |
| 0.897578152 | 0.503215187 | 0.498522748 |
| 0.897411135 | 0.627589246 | 0.495546921 |
| 0.960246234 | 0.314665411 | 0.501525530 |
| 0.960109670 | 0.440234649 | 0.501094351 |

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| 0.960469971 | 0.565844547 | 0.496189782 |
| 0.957038357 | 0.691627382 | 0.488481587 |
| 0.022740323 | 0.293650488 | 0.502056048 |
| 0.022664517 | 0.419265440 | 0.502851431 |
| 0.022616122 | 0.544593500 | 0.497691711 |
| 0.023501821 | 0.672733784 | 0.490259104 |
| 0.085173806 | 0.356440561 | 0.504242345 |
| 0.085206359 | 0.482002711 | 0.502754748 |
| 0.084576422 | 0.607353353 | 0.492452646 |
| 0.110894961 | 0.731038683 | 0.500227691 |
| 0.147717298 | 0.293652081 | 0.503373977 |
| 0.147656379 | 0.419180414 | 0.506093672 |
| 0.147763656 | 0.544890420 | 0.500950277 |
| 0.148488885 | 0.667507464 | 0.485965538 |
| 0.210199674 | 0.356410643 | 0.506249198 |
| 0.210085117 | 0.481934196 | 0.507096529 |
| 0.211384808 | 0.607394287 | 0.498154780 |
| 0.181448669 | 0.731632193 | 0.507412486 |
| 0.272729098 | 0.293627549 | 0.504085838 |
| 0.272683133 | 0.419170139 | 0.508510696 |
| 0.272690960 | 0.544496249 | 0.507817976 |
| 0.273023663 | 0.673334767 | 0.494995080 |
| 0.335229330 | 0.356374929 | 0.506644722 |
| 0.335227784 | 0.481922877 | 0.510248256 |
| 0.334264103 | 0.607608186 | 0.509337969 |
| 0.370349695 | 0.729166504 | 0.455729522 |
| 0.397759563 | 0.293608868 | 0.503733213 |
| 0.397697063 | 0.419120277 | 0.508131813 |
| 0.397603371 | 0.544942453 | 0.511335679 |
| 0.397690544 | 0.667975426 | 0.507680165 |
| 0.460264554 | 0.356382704 | 0.504936870 |
| 0.460067844 | 0.481907493 | 0.508550527 |
| 0.460992769 | 0.607529011 | 0.509311204 |
| 0.435850792 | 0.729872651 | 0.458028225 |
| 0.522767284 | 0.293594829 | 0.502264978 |
| 0.522700286 | 0.419172639 | 0.504773212 |
| 0.522517519 | 0.544446799 | 0.506261410 |
| 0.522486828 | 0.673178505 | 0.495001312 |
| 0.585243177 | 0.356386550 | 0.502010333 |
| 0.585208108 | 0.481922657 | 0.503266886 |
| 0.583823909 | 0.607357145 | 0.498320462 |
| 0.619468190 | 0.732014057 | 0.500441081 |
| 0.647765178 | 0.293603181 | 0.500724927 |
| 0.647711647 | 0.419159920 | 0.500962014 |
| 0.647501424 | 0.544906739 | 0.499428322 |
| 0.646950837 | 0.667304774 | 0.487332694 |

| | | |
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| 0.710254871 | 0.356400451 | 0.500034105 |
| 0.710090470 | 0.481985129 | 0.499440407 |
| 0.710784235 | 0.607416759 | 0.493056752 |
| 0.684954394 | 0.732295373 | 0.499172316 |
| 0.772774302 | 0.293615900 | 0.500088520 |
| 0.772707591 | 0.419227144 | 0.499519784 |
| 0.772614851 | 0.544593995 | 0.496943499 |
| 0.771580675 | 0.673404437 | 0.490340632 |
| 0.835233065 | 0.356425671 | 0.500096619 |
| 0.835225738 | 0.482030074 | 0.498741043 |
| 0.833958594 | 0.607841590 | 0.494872550 |
| 0.862989745 | 0.730920003 | 0.486093953 |
| 0.897764298 | 0.293643565 | 0.500684369 |
| 0.897693970 | 0.419217694 | 0.500382300 |
| 0.897519529 | 0.545125473 | 0.497029330 |
| 0.897487744 | 0.668257182 | 0.495637751 |
| 0.960219778 | 0.356449571 | 0.501763059 |
| 0.960030111 | 0.482062106 | 0.499945142 |
| 0.960957510 | 0.607670493 | 0.494424920 |
| 0.934443611 | 0.730058253 | 0.478485286 |
| 0.085267278 | 0.232837291 | 0.500674909 |
| 0.210253086 | 0.232838719 | 0.501027407 |
| 0.335255763 | 0.232816604 | 0.501275725 |
| 0.460275879 | 0.232792044 | 0.501249182 |
| 0.585284432 | 0.232767484 | 0.501024718 |
| 0.710291129 | 0.232798582 | 0.500738563 |
| 0.835299587 | 0.232806412 | 0.500474933 |
| 0.960292580 | 0.232822730 | 0.500449655 |
| 0.832729327 | 0.761086178 | 0.440650474 |
| 0.335418855 | 0.755264040 | 0.423264973 |
| 0.211290521 | 0.762247924 | 0.525692330 |
| 0.584509204 | 0.761471888 | 0.510098266 |
| 0.077632642 | 0.761614909 | 0.509662816 |
| 0.958466618 | 0.755655629 | 0.486598276 |
| 0.780099849 | 0.780499386 | 0.550684631 |
| 0.900703329 | 0.793525022 | 0.584636240 |
| 0.906242122 | 0.824518332 | 0.489549331 |
| 0.855446648 | 0.837227103 | 0.581837136 |
| 0.728933035 | 0.803391405 | 0.412271605 |
| 0.753363450 | 0.843817365 | 0.477259453 |
| 0.802679702 | 0.829943716 | 0.384089200 |
| 0.812629088 | 0.793033654 | 0.499291049 |
| 0.872568838 | 0.812953010 | 0.540785836 |
| 0.771995554 | 0.819044926 | 0.439198310 |

IM9'
E+ZPE = -1200.67 eV
1.0
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     0.0000000000         34.7140998840          0.0000000000
     0.0000000000          0.0000000000         15.0721998215
   B   N   O   H
  64   64   13    1
Direct
    0.015177999          0.253526997          0.509123977
    0.015167999          0.379200987          0.505649996
    0.015163000          0.504534020          0.496482012
    0.015441000          0.631025035          0.480504984
    0.077664005          0.316430997          0.508665970
    0.077702001          0.441924989          0.503821006
    0.077373997          0.567202995          0.489789012
    0.081036003          0.691641998          0.475937000
    0.140156000          0.253524991          0.509789996
    0.140155000          0.379162004          0.508351974
    0.140200002          0.504733963          0.500591989
    0.140645001          0.628332040          0.480088010
    0.202678988          0.316417014          0.510139995
    0.202632999          0.441902022          0.507557984
    0.203278015          0.567226016          0.495947982
    0.199659993          0.692403968          0.478082011
    0.265162994          0.253504003          0.510236013
    0.265172011          0.379166015          0.510391002
    0.265206985          0.504490009          0.505851998
    0.265390014          0.631096023          0.489858012
    0.327684996          0.316403003          0.510709996
    0.327732008          0.441904000          0.509868013
    0.327288008          0.567394037          0.502786986
    0.332132013          0.691055025          0.473512003
    0.390171000          0.253496997          0.510221017
    0.390206997          0.379132993          0.510523972
    0.390213992          0.504804017          0.507269013
    0.390410987          0.628857035          0.499208003
    0.452697998          0.316395997          0.510049988
    0.452668020          0.441896995          0.508279020
    0.453183014          0.567397004          0.501366017
    0.449081000          0.693032972          0.471242026
    0.515191021          0.253497986          0.509725995
    0.515223996          0.379159999          0.508306038
    0.515182028          0.504472042          0.502829000
    0.515081008          0.631314977          0.488990023
    0.577715972          0.316400997          0.508386016

| | | |
|---|---|---|
| 0.577767029 | 0.441895978 | 0.504002981 |
| 0.577125035 | 0.567264972 | 0.494078022 |
| 0.581143018 | 0.691488043 | 0.476620989 |
| 0.640219987 | 0.253502025 | 0.509024036 |
| 0.640228980 | 0.379142993 | 0.505190028 |
| 0.640181016 | 0.504783962 | 0.497550010 |
| 0.640021993 | 0.628356985 | 0.482154024 |
| 0.702732995 | 0.316406025 | 0.506752003 |
| 0.702676990 | 0.441922984 | 0.500464967 |
| 0.703143021 | 0.567377993 | 0.489456002 |
| 0.698461013 | 0.693801975 | 0.477719010 |
| 0.765218976 | 0.253509992 | 0.508582006 |
| 0.765209031 | 0.379180987 | 0.503264007 |
| 0.765209983 | 0.504571986 | 0.494735974 |
| 0.764800005 | 0.631816016 | 0.481992992 |
| 0.827709953 | 0.316424019 | 0.506228033 |
| 0.827736980 | 0.441949989 | 0.499301996 |
| 0.827139048 | 0.567614968 | 0.487844990 |
| 0.830626049 | 0.692875007 | 0.478127980 |
| 0.890207972 | 0.253520019 | 0.508631992 |
| 0.890195030 | 0.379171015 | 0.503539026 |
| 0.890140023 | 0.504891983 | 0.494363987 |
| 0.890130031 | 0.629064011 | 0.481781974 |
| 0.952691051 | 0.316430997 | 0.507047998 |
| 0.952620056 | 0.441962983 | 0.500706008 |
| 0.953095985 | 0.567418981 | 0.487825976 |
| 0.950130021 | 0.693169015 | 0.477666999 |
| 0.015180001 | 0.295437997 | 0.508346976 |
| 0.015158001 | 0.421030999 | 0.503551017 |
| 0.015205000 | 0.546265022 | 0.491356998 |
| 0.016065999 | 0.674314977 | 0.477553992 |
| 0.077656000 | 0.358229993 | 0.507767989 |
| 0.077735999 | 0.483747968 | 0.500522008 |
| 0.077182004 | 0.608951963 | 0.482647970 |
| 0.103620995 | 0.732698995 | 0.482540025 |
| 0.140167003 | 0.295439975 | 0.509683001 |
| 0.140157998 | 0.420976000 | 0.506901993 |
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| 0.390293979 | 0.669660958 | 0.492226980 |
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| 0.577755990 | 0.483721980 | 0.501485003 |
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| 0.611476001 | 0.733782006 | 0.480387010 |
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| 0.827772002 | 0.483775001 | 0.496104996 |
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| 0.462747974 | 0.483295995 | 0.501757017 |
| 0.463685984 | 0.608798009 | 0.497671021 |
| 0.438905022 | 0.731191978 | 0.449927004 |
| 0.525326029 | 0.294990007 | 0.508363016 |
| 0.525319986 | 0.420547982 | 0.502321007 |
| 0.525265979 | 0.545827993 | 0.495027982 |
| 0.524932039 | 0.674337999 | 0.485876006 |
| 0.587822954 | 0.357773019 | 0.504251014 |
| 0.587831043 | 0.483276984 | 0.495707004 |
| 0.586597969 | 0.608776965 | 0.483873994 |
| 0.618973038 | 0.731359009 | 0.510927025 |

| | | |
|---|---|---|
| 0.650326017 | 0.294998002 | 0.507038000 |
| 0.650298990 | 0.420513999 | 0.498542996 |
| 0.650151006 | 0.546227989 | 0.487361990 |
| 0.649792037 | 0.669062008 | 0.473998008 |
| 0.712819992 | 0.357774997 | 0.502377985 |
| 0.712694990 | 0.483304017 | 0.492081989 |
| 0.713448996 | 0.608757954 | 0.480340978 |
| 0.686171004 | 0.731069012 | 0.513124997 |
| 0.775312016 | 0.294998002 | 0.506416020 |
| 0.775275995 | 0.420565015 | 0.497249016 |
| 0.775266003 | 0.545894971 | 0.486980006 |
| 0.774496009 | 0.674503986 | 0.485311003 |
| 0.837792953 | 0.357779997 | 0.502247989 |
| 0.837845009 | 0.483329017 | 0.492667998 |
| 0.836781998 | 0.609050973 | 0.486658987 |
| 0.864413057 | 0.731676973 | 0.474350981 |
| 0.900292019 | 0.295003002 | 0.506750991 |
| 0.900268988 | 0.420533010 | 0.498373992 |
| 0.900245006 | 0.546339966 | 0.489883005 |
| 0.900425062 | 0.669363983 | 0.492119004 |
| 0.962786993 | 0.357777003 | 0.503489958 |
| 0.962702961 | 0.483319017 | 0.495148012 |
| 0.963779961 | 0.608838009 | 0.488856990 |
| 0.935963993 | 0.731379998 | 0.475822981 |
| 0.087765003 | 0.234184008 | 0.510915984 |
| 0.212774003 | 0.234174008 | 0.511200020 |
| 0.337797996 | 0.234167002 | 0.511273038 |
| 0.462821015 | 0.234167991 | 0.511098972 |
| 0.587829996 | 0.234181013 | 0.510773017 |
| 0.712823989 | 0.234189008 | 0.510538999 |
| 0.837797996 | 0.234191013 | 0.510492018 |
| 0.962769006 | 0.234184008 | 0.510636979 |
| 0.834013029 | 0.763422033 | 0.453326987 |
| 0.213757002 | 0.764052961 | 0.511707001 |
| 0.585380027 | 0.759439986 | 0.538103979 |
| 0.338779997 | 0.756663036 | 0.413383008 |
| 0.079887003 | 0.763021982 | 0.496586003 |
| 0.958587004 | 0.757474017 | 0.468945000 |
| 0.844787985 | 0.796495981 | 0.589718006 |
| 0.865341027 | 0.835002016 | 0.453032985 |
| 0.777387981 | 0.840137018 | 0.435141009 |
| 0.816878944 | 0.865884008 | 0.522117016 |
| 0.716835976 | 0.765839975 | 0.539029990 |
| 0.731975988 | 0.787228988 | 0.645578966 |
| 0.697972998 | 0.817374998 | 0.555747985 |
| 0.802739942 | 0.806842029 | 0.550103019 |

```
     0.816812993        0.838231049        0.485698998
     0.737712965        0.797791023        0.577371023



IM10
E+ZPE = -1251.43490 eV
1.0
      20.0422000885        0.0000000000        0.0000000000
       0.0000000000       34.7140998840        0.0000000000
       0.0000000000        0.0000000000       15.0721998215
    B   N   O   H   C
   64  64  13   8   3
Direct
     0.025212989        0.251710999        0.504834841
     0.025197233        0.377349990        0.497978025
     0.025262080        0.502631347        0.490181372
     0.025457701        0.629312250        0.487737045
     0.087700302        0.314601977        0.502745637
     0.087775531        0.440052343        0.496051751
     0.087483548        0.565427134        0.488369466
     0.090901351        0.689957344        0.495101126
     0.150234788        0.251715065        0.505652622
     0.150203466        0.377318809        0.501658215
     0.150295814        0.502884586        0.495193221
     0.150655091        0.626799748        0.487328739
     0.212713596        0.314611180        0.505103533
     0.212677266        0.440054926        0.501650211
     0.213298894        0.565446364        0.496457715
     0.209356759        0.690762061        0.498736993
     0.275256510        0.251735147        0.506564491
     0.275226865        0.377360429        0.505262793
     0.275209973        0.502650303        0.503216014
     0.275204121        0.629406974        0.500784468
     0.337744108        0.314629724        0.506626911
     0.337758193        0.440113826        0.506071684
     0.337161237        0.565554385        0.507323966
     0.341818073        0.689844653        0.496365399
     0.400276459        0.251750257        0.507023922
     0.400254809        0.377384770        0.506451674
     0.400209081        0.503045628        0.507940537
     0.400064713        0.627006175        0.513395966
     0.462760727        0.314664889        0.506277672
     0.462702675        0.440191628        0.506023659
     0.463111797        0.565741416        0.509736783
     0.458724282        0.691748480        0.496054883
     0.525270642        0.251758691        0.506684490
```

| | | |
|---|---|---|
| 0.525255320 | 0.377452434 | 0.504442385 |
| 0.525233051 | 0.502886069 | 0.505358621 |
| 0.524828260 | 0.630063891 | 0.505881072 |
| 0.587735543 | 0.314666427 | 0.504208621 |
| 0.587754767 | 0.440235446 | 0.501937916 |
| 0.587134852 | 0.565935810 | 0.502974403 |
| 0.590374133 | 0.691107223 | 0.499395546 |
| 0.650237084 | 0.251761163 | 0.505851396 |
| 0.650209152 | 0.377422956 | 0.500687469 |
| 0.650120933 | 0.503209088 | 0.499023718 |
| 0.649976851 | 0.627442379 | 0.497232091 |
| 0.712713786 | 0.314650740 | 0.501813172 |
| 0.712608865 | 0.440233825 | 0.496945904 |
| 0.712994052 | 0.565862733 | 0.495272282 |
| 0.709775754 | 0.691609415 | 0.498143802 |
| 0.775215802 | 0.251746768 | 0.504963887 |
| 0.775168362 | 0.377411390 | 0.497519037 |
| 0.775102744 | 0.502870630 | 0.493176118 |
| 0.775119541 | 0.629805706 | 0.493202566 |
| 0.837705209 | 0.314623213 | 0.500455508 |
| 0.837667142 | 0.440153029 | 0.493513873 |
| 0.837218146 | 0.565709164 | 0.489667526 |
| 0.841063164 | 0.690338055 | 0.497166254 |
| 0.900210461 | 0.251724131 | 0.504529545 |
| 0.900180674 | 0.377349742 | 0.496438258 |
| 0.900144606 | 0.502997717 | 0.489702200 |
| 0.900388518 | 0.627029471 | 0.488937189 |
| 0.962709813 | 0.314610164 | 0.500843470 |
| 0.962646146 | 0.440083085 | 0.492976964 |
| 0.963218383 | 0.565498397 | 0.486935620 |
| 0.960074934 | 0.691374967 | 0.496436265 |
| 0.025204950 | 0.293607879 | 0.502799799 |
| 0.025211187 | 0.419157612 | 0.495242163 |
| 0.025370858 | 0.544398447 | 0.487689463 |
| 0.025943690 | 0.672642411 | 0.492795843 |
| 0.087687032 | 0.356385149 | 0.500757039 |
| 0.087854228 | 0.481866669 | 0.493271661 |
| 0.087235621 | 0.607317640 | 0.486198639 |
| 0.112986629 | 0.730528853 | 0.511483486 |
| 0.150209831 | 0.293619279 | 0.504614458 |
| 0.150216564 | 0.419117695 | 0.499805465 |
| 0.150417615 | 0.544801190 | 0.492452203 |
| 0.150937391 | 0.667657078 | 0.486574738 |
| 0.212714809 | 0.356397264 | 0.504256424 |
| 0.212663252 | 0.481883097 | 0.500085546 |
| 0.213883669 | 0.607371265 | 0.494081375 |

| | | |
|---|---|---|
| 0.183548914 | 0.731142803 | 0.518405917 |
| 0.275238214 | 0.293634417 | 0.506304215 |
| 0.275211044 | 0.419182419 | 0.504743505 |
| 0.275196721 | 0.544448172 | 0.502675878 |
| 0.275213447 | 0.673319602 | 0.498582700 |
| 0.337742776 | 0.356418720 | 0.506480148 |
| 0.337769351 | 0.481949690 | 0.506431395 |
| 0.336546722 | 0.607514176 | 0.508753130 |
| 0.372337821 | 0.729788586 | 0.465747462 |
| 0.400260043 | 0.293655845 | 0.506908954 |
| 0.400235252 | 0.419193326 | 0.506617483 |
| 0.400093929 | 0.544971244 | 0.509715745 |
| 0.399651357 | 0.667853394 | 0.512126569 |
| 0.462771719 | 0.356457703 | 0.505997970 |
| 0.462655235 | 0.482029414 | 0.506996208 |
| 0.463371316 | 0.607585054 | 0.511637273 |
| 0.437807513 | 0.730520446 | 0.468339565 |
| 0.525255082 | 0.293662081 | 0.505816406 |
| 0.525234764 | 0.419275413 | 0.504245889 |
| 0.525158726 | 0.544665533 | 0.506610618 |
| 0.524219098 | 0.673356745 | 0.501262785 |
| 0.587724076 | 0.356460808 | 0.503068206 |
| 0.587753244 | 0.482074799 | 0.502101352 |
| 0.586499139 | 0.607843074 | 0.502377795 |
| 0.615277575 | 0.731498129 | 0.505129918 |
| 0.650224189 | 0.293659883 | 0.503839671 |
| 0.650184457 | 0.419239342 | 0.499588246 |
| 0.650036282 | 0.545138385 | 0.499006096 |
| 0.649825916 | 0.668220039 | 0.495833235 |
| 0.712692992 | 0.356435945 | 0.499688725 |
| 0.712535967 | 0.482079084 | 0.496064058 |
| 0.713346739 | 0.607688240 | 0.494847810 |
| 0.686878092 | 0.730560171 | 0.503164477 |
| 0.775210568 | 0.293634307 | 0.502160861 |
| 0.775129724 | 0.419237611 | 0.495579412 |
| 0.775095654 | 0.544643720 | 0.492312685 |
| 0.775415319 | 0.672842190 | 0.496075826 |
| 0.837672757 | 0.356406605 | 0.497743943 |
| 0.837683511 | 0.481985843 | 0.491642964 |
| 0.836941782 | 0.607571703 | 0.489821851 |
| 0.865546397 | 0.730789894 | 0.504566908 |
| 0.900210176 | 0.293617164 | 0.501738003 |
| 0.900158690 | 0.419150744 | 0.493858114 |
| 0.900203609 | 0.544908717 | 0.487942210 |
| 0.900683249 | 0.667826472 | 0.492102584 |
| 0.962700201 | 0.356388446 | 0.498119726 |

```
0.962630158        0.481904306        0.490344682
0.963818599        0.607367969        0.486766078
0.936655949        0.730265064        0.503756150
0.087723303        0.232798445        0.505834755
0.212750520        0.232817044        0.506379542
0.337771778        0.232830725        0.506949892
0.462780474        0.232840533        0.507149742
0.587759145        0.232833527        0.506988932
0.712726300        0.232843142        0.506538929
0.837705780        0.232825560        0.505953742
0.962710289        0.232802621        0.505652970
0.834627806        0.762564185        0.511687386
0.337166376        0.756520126        0.436047722
0.213109869        0.761179034        0.541407500
0.585783200        0.763315880        0.513790130
0.079169964        0.760592666        0.526048182
0.959699597        0.756277985        0.511064582
0.749533850        0.863442220        0.577294082
0.863570071        0.839326642        0.521317648
0.862797223        0.876226869        0.438820693
0.868969636        0.888212077        0.553657737
0.709280412        0.756884737        0.506691577
0.675465472        0.879614417        0.454758175
0.748361540        0.886068582        0.379505493
0.770889384        0.870205942        0.512124291
0.845312639        0.868507608        0.505662556
0.729477578        0.879045961        0.445655521
```

IM11
E+ZPE = -1204.89035 eV
1.0
```
    20.0422000885        0.0000000000        0.0000000000
     0.0000000000       34.7140998840        0.0000000000
     0.0000000000        0.0000000000       15.0721998215
   B   N   O   H
  64  64  13   2
Direct
  0.022858629        0.251669324        0.501487724
  0.022875372        0.377292353        0.500877132
  0.022927327        0.502595138        0.495132036
  0.023092959        0.629290547        0.488133296
  0.085384630        0.314545659        0.502670594
  0.085432933        0.439995696        0.500544913
  0.085099606        0.565379167        0.491907290
  0.088539785        0.689974762        0.491230261
```

| | | |
|---|---|---|
| 0.147902908 | 0.251661384 | 0.502289465 |
| 0.147886599 | 0.377260238 | 0.504194321 |
| 0.147928710 | 0.502833268 | 0.499686415 |
| 0.148270513 | 0.626693156 | 0.487940438 |
| 0.210420246 | 0.314549093 | 0.504827153 |
| 0.210350180 | 0.440017234 | 0.505421103 |
| 0.210914137 | 0.565387793 | 0.499365618 |
| 0.207054036 | 0.690748160 | 0.494617525 |
| 0.272929400 | 0.251667428 | 0.502981237 |
| 0.272898114 | 0.377309358 | 0.507312355 |
| 0.272877606 | 0.502616512 | 0.506859727 |
| 0.272850459 | 0.629360271 | 0.500277329 |
| 0.335409695 | 0.314579175 | 0.505914733 |
| 0.335435770 | 0.440064953 | 0.509340879 |
| 0.334828131 | 0.565553011 | 0.509242900 |
| 0.339481566 | 0.689688995 | 0.491683111 |
| 0.397915922 | 0.251704213 | 0.503194090 |
| 0.397913638 | 0.377333396 | 0.508013302 |
| 0.397860202 | 0.503025354 | 0.511051833 |
| 0.397732322 | 0.627048097 | 0.512186932 |
| 0.460409207 | 0.314617307 | 0.505196798 |
| 0.460365621 | 0.440160447 | 0.509028307 |
| 0.460787970 | 0.565744438 | 0.511007067 |
| 0.456363531 | 0.691570295 | 0.490894752 |
| 0.522894569 | 0.251729350 | 0.502731559 |
| 0.522899232 | 0.377408973 | 0.505771830 |
| 0.522885957 | 0.502859751 | 0.508325874 |
| 0.522478453 | 0.630037407 | 0.504117475 |
| 0.585382453 | 0.314644916 | 0.503067447 |
| 0.585408672 | 0.440211655 | 0.505024662 |
| 0.584793324 | 0.565899491 | 0.504283663 |
| 0.588005008 | 0.691011619 | 0.494276606 |
| 0.647869100 | 0.251738526 | 0.501817063 |
| 0.647858156 | 0.377417324 | 0.502319109 |
| 0.647801770 | 0.503181121 | 0.502311041 |
| 0.647635038 | 0.627336501 | 0.496028308 |
| 0.710357984 | 0.314651372 | 0.500974194 |
| 0.710290606 | 0.440222836 | 0.500501571 |
| 0.710689925 | 0.565807240 | 0.497195677 |
| 0.707400014 | 0.691472109 | 0.493123189 |
| 0.772843441 | 0.251720724 | 0.501154366 |
| 0.772838112 | 0.377418725 | 0.499727448 |
| 0.772813559 | 0.502840795 | 0.497066503 |
| 0.772808657 | 0.629729883 | 0.492445401 |
| 0.835327185 | 0.314614999 | 0.500114367 |
| 0.835370105 | 0.440148222 | 0.497632898 |

| | | |
|---|---|---|
| 0.834924250 | 0.565661801 | 0.492457613 |
| 0.838616810 | 0.690351406 | 0.492505385 |
| 0.897833770 | 0.251704845 | 0.501033355 |
| 0.897838433 | 0.377330484 | 0.499159756 |
| 0.897864223 | 0.502972607 | 0.494296854 |
| 0.898061123 | 0.627001010 | 0.489323380 |
| 0.960358055 | 0.314574807 | 0.500771655 |
| 0.960338260 | 0.440048854 | 0.497586613 |
| 0.960888990 | 0.565467463 | 0.490409474 |
| 0.957622871 | 0.691496559 | 0.492066803 |
| 0.022868452 | 0.293570901 | 0.501630437 |
| 0.022881656 | 0.419104810 | 0.499603685 |
| 0.023003166 | 0.544353228 | 0.492021657 |
| 0.023529377 | 0.672691587 | 0.490103419 |
| 0.085376041 | 0.356327375 | 0.502716721 |
| 0.085493899 | 0.481815570 | 0.498289838 |
| 0.084839224 | 0.607243574 | 0.488014310 |
| 0.110785008 | 0.730765389 | 0.504055087 |
| 0.147906358 | 0.293561560 | 0.503442945 |
| 0.147893962 | 0.419065635 | 0.503580028 |
| 0.148016299 | 0.544742784 | 0.496451483 |
| 0.148544783 | 0.667512244 | 0.484750082 |
| 0.210403616 | 0.356334683 | 0.505856205 |
| 0.210322463 | 0.481844416 | 0.504216846 |
| 0.211484590 | 0.607291321 | 0.495393925 |
| 0.181380090 | 0.731418899 | 0.510848408 |
| 0.272924356 | 0.293566340 | 0.504840504 |
| 0.272887979 | 0.419132859 | 0.507943384 |
| 0.272849222 | 0.544417788 | 0.505707132 |
| 0.272873466 | 0.673238779 | 0.495319389 |
| 0.335405198 | 0.356363364 | 0.507566336 |
| 0.335432416 | 0.481907712 | 0.509961183 |
| 0.334210643 | 0.607522033 | 0.508957757 |
| 0.369961986 | 0.729208811 | 0.458238705 |
| 0.397914923 | 0.293603263 | 0.505033678 |
| 0.397911568 | 0.419142392 | 0.509446800 |
| 0.397772102 | 0.544969266 | 0.511976673 |
| 0.397319775 | 0.667876581 | 0.508693621 |
| 0.460414869 | 0.356403391 | 0.506594546 |
| 0.460308949 | 0.482001887 | 0.510271415 |
| 0.461033595 | 0.607606538 | 0.511072587 |
| 0.435437626 | 0.729979408 | 0.460701540 |
| 0.522895235 | 0.293629362 | 0.503775765 |
| 0.522889716 | 0.419238545 | 0.506871590 |
| 0.522825716 | 0.544646027 | 0.508607315 |
| 0.521872146 | 0.673273504 | 0.497095451 |

| | | |
|---|---|---|
| 0.585376315 | 0.356436797 | 0.503694711 |
| 0.585418284 | 0.482050128 | 0.505465806 |
| 0.584151045 | 0.607792030 | 0.501879040 |
| 0.612942804 | 0.731472140 | 0.497135250 |
| 0.647872431 | 0.293642988 | 0.501773183 |
| 0.647847830 | 0.419230908 | 0.502574450 |
| 0.647728158 | 0.545104539 | 0.501329191 |
| 0.647451557 | 0.668084326 | 0.492406045 |
| 0.710349371 | 0.356442868 | 0.500792314 |
| 0.710231126 | 0.482059799 | 0.499928153 |
| 0.711041328 | 0.607612746 | 0.494970055 |
| 0.684508205 | 0.730455941 | 0.495240328 |
| 0.772836256 | 0.293623895 | 0.500526437 |
| 0.772823789 | 0.419243298 | 0.499092813 |
| 0.772813701 | 0.544600863 | 0.495401582 |
| 0.773043624 | 0.672763729 | 0.492509877 |
| 0.835321761 | 0.356403528 | 0.499470336 |
| 0.835397989 | 0.481971613 | 0.496070417 |
| 0.834655594 | 0.607511484 | 0.490839609 |
| 0.862868789 | 0.730934563 | 0.495838392 |
| 0.897836054 | 0.293603455 | 0.500478033 |
| 0.897839670 | 0.419135249 | 0.497921236 |
| 0.897910284 | 0.544870201 | 0.491910453 |
| 0.898292092 | 0.667821417 | 0.489939477 |
| 0.960356152 | 0.356358199 | 0.500171314 |
| 0.960323795 | 0.481869251 | 0.495373362 |
| 0.961486446 | 0.607329617 | 0.488484497 |
| 0.934047908 | 0.730471656 | 0.495461407 |
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| 0.657356975 | 0.627538037 | 0.496313008 |
| 0.719810028 | 0.315203015 | 0.495786001 |
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   0.157279997        0.503648974        0.503707999
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   0.469772033        0.440720001        0.499840993
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| 0.782208028 | 0.630491029 | 0.498559004 |
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| 0.844852984 | 0.440737007 | 0.498345993 |
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| 0.907286956 | 0.503667984 | 0.500450003 |
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| 0.969847976 | 0.315207987 | 0.498194010 |
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| 0.157251995 | 0.545632006 | 0.503591006 |
| 0.157298995 | 0.668321027 | 0.500256006 |
| 0.219828990 | 0.357000994 | 0.501246999 |
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| 0.220764002 | 0.608163015 | 0.502262004 |
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| 0.532340000 | 0.674229978 | 0.500594963 |
| 0.594809993 | 0.357019016 | 0.496610996 |
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| 0.907279058 | 0.545639973 | 0.501053982 |
| 0.907258977 | 0.668323994 | 0.503404032 |
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| 0.969837032 | 0.233427999 | 0.496196015 |
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| 0.094846168 | 0.440734919 | 0.502628454 |
| 0.094284221 | 0.566294652 | 0.503237432 |
| 0.098592295 | 0.690885522 | 0.501083025 |
| 0.157323929 | 0.252309592 | 0.497511254 |
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| 0.157387357 | 0.627550510 | 0.501544607 |
| 0.219822852 | 0.315206009 | 0.499841721 |
| 0.219757306 | 0.440736430 | 0.503100634 |
| 0.220313507 | 0.566280147 | 0.503184852 |
| 0.216137025 | 0.693065499 | 0.501229598 |
| 0.282324393 | 0.252305471 | 0.497433111 |
| 0.282311093 | 0.377977318 | 0.501401893 |
| 0.282300982 | 0.503341120 | 0.503277611 |
| 0.282275977 | 0.630513172 | 0.501948546 |

| 0.344818320 | 0.315207603 | 0.499110909 |
| 0.344861454 | 0.440729617 | 0.502011883 |
| 0.344285839 | 0.566272180 | 0.502436513 |
| 0.348662290 | 0.690887170 | 0.501222860 |
| 0.407323929 | 0.252310526 | 0.496859978 |
| 0.407312699 | 0.377952429 | 0.499854470 |
| 0.407300327 | 0.503658534 | 0.501506579 |
| 0.407401585 | 0.627531334 | 0.502068988 |
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| 0.782310474 | 0.503357109 | 0.497860146 |
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| 0.157282436 | 0.545639314 | 0.503593758 |
| 0.157289657 | 0.668299379 | 0.500223862 |
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| 0.407322596 | 0.294228064 | 0.497921426 |
| 0.407313460 | 0.419776562 | 0.500707622 |
| 0.407285196 | 0.545615193 | 0.501608418 |
| 0.407331352 | 0.668284819 | 0.502545407 |
| 0.469818427 | 0.357016269 | 0.498451565 |
| 0.469724545 | 0.482591881 | 0.500150623 |
| 0.470812062 | 0.608135763 | 0.500548425 |
| 0.445585815 | 0.733506625 | 0.498355010 |
| 0.532325249 | 0.294225812 | 0.496595051 |
| 0.532304360 | 0.419824253 | 0.498329795 |
| 0.532309832 | 0.545140363 | 0.498657553 |
| 0.532428457 | 0.674194099 | 0.500761404 |
| 0.594807185 | 0.357021928 | 0.496740612 |
| 0.594885603 | 0.482591936 | 0.497546909 |
| 0.593796183 | 0.608229498 | 0.496502197 |
| 0.629868380 | 0.733036080 | 0.511552739 |
| 0.657329377 | 0.294233696 | 0.495821055 |
| 0.657306204 | 0.419783073 | 0.496737733 |
| 0.657277035 | 0.545628984 | 0.496461290 |
| 0.657307869 | 0.668337785 | 0.495331886 |
| 0.719826873 | 0.357024730 | 0.496221704 |
| 0.719722665 | 0.482597101 | 0.496939639 |
| 0.720781489 | 0.608168510 | 0.496243027 |
| 0.695519317 | 0.733254979 | 0.511030794 |

```
0.782328984        0.294230042        0.496060514
0.782309475        0.419829253        0.497214943
0.782315471        0.545155308        0.497964516
0.782400407        0.674195198        0.499372451
0.844812538        0.357024153        0.497326748
0.844892193        0.482596991        0.498902992
0.843796349        0.608227355        0.500656054
0.879740024        0.733158771        0.492280288
0.907327117        0.294231691        0.497117976
0.907310653        0.419785353        0.499294688
0.907290478        0.545632226        0.501157688
0.907282484        0.668308774        0.503427443
0.969818760        0.357015252        0.499226953
0.969722546        0.482601057        0.501486110
0.970784892        0.608170433        0.502980477
0.945385965        0.733435966        0.493031221
0.094825285        0.233412917        0.496685469
0.219823566        0.233410582        0.496802905
0.344823816        0.233412972        0.496583820
0.469822043        0.233411131        0.496144637
0.594830501        0.233413823        0.495709630
0.719827349        0.233414593        0.495564417
0.844827194        0.233414043        0.495812481
0.969824851        0.233414016        0.496283238
0.844988311        0.762650173        0.484874256
0.595198035        0.762437483        0.521165379
0.095033759        0.762985060        0.505543696
0.345262581        0.762985664        0.496197122
```

IM15
E+ZPE = -1245.05308 eV
1.0
```
    20.0422000885        0.0000000000        0.0000000000
     0.0000000000       34.7140998840        0.0000000000
     0.0000000000        0.0000000000       15.0721998215
```
  B   N   O   H   C
 64  64  12   8   3
Direct
```
  0.021124999        0.249510005        0.504357978
  0.021114999        0.375178995        0.500087982
  0.021081001        0.500529006        0.495983985
  0.020962000        0.627638970        0.492148995
  0.083635004        0.312411011        0.502650030
  0.083630001        0.437932008        0.498948992
  0.083047005        0.563451000        0.493740994
```

| | | |
|---|---|---|
| 0.087323002 | 0.687994013 | 0.490895986 |
| 0.146107007 | 0.249502011 | 0.504721992 |
| 0.146109993 | 0.375155974 | 0.501897990 |
| 0.146066989 | 0.500855980 | 0.497547004 |
| 0.146091994 | 0.624701033 | 0.489183988 |
| 0.208632018 | 0.312418016 | 0.504074986 |
| 0.208520982 | 0.437943986 | 0.501268986 |
| 0.209046016 | 0.563451989 | 0.495426005 |
| 0.204841007 | 0.690153002 | 0.491164013 |
| 0.271116000 | 0.249512999 | 0.505218976 |
| 0.271086998 | 0.375203995 | 0.503890986 |
| 0.271055997 | 0.500567961 | 0.500191972 |
| 0.270945985 | 0.627638970 | 0.493858019 |
| 0.333626986 | 0.312427027 | 0.505133999 |
| 0.333604003 | 0.437962008 | 0.503266981 |
| 0.333027008 | 0.563498966 | 0.499055007 |
| 0.337314003 | 0.687925992 | 0.489622001 |
| 0.396120984 | 0.249516983 | 0.505419015 |
| 0.396097002 | 0.375178006 | 0.504746004 |
| 0.396046017 | 0.500889991 | 0.501790995 |
| 0.396073020 | 0.624786966 | 0.498978003 |
| 0.458644009 | 0.312436010 | 0.505071991 |
| 0.458523004 | 0.437956980 | 0.503256035 |
| 0.459035001 | 0.563481989 | 0.499168994 |
| 0.454794994 | 0.690096958 | 0.489063009 |
| 0.521143027 | 0.249532010 | 0.505231978 |
| 0.521110005 | 0.375207979 | 0.503801992 |
| 0.521058995 | 0.500565983 | 0.500151984 |
| 0.520950029 | 0.627644025 | 0.494096023 |
| 0.583642998 | 0.312438016 | 0.504043982 |
| 0.583617969 | 0.437949013 | 0.500944962 |
| 0.583024986 | 0.563463967 | 0.495470993 |
| 0.587278030 | 0.687970002 | 0.490808984 |
| 0.646151009 | 0.249529016 | 0.504848002 |
| 0.646109993 | 0.375167018 | 0.501567006 |
| 0.646053035 | 0.500851969 | 0.497099026 |
| 0.646058032 | 0.624689000 | 0.489170005 |
| 0.708652027 | 0.312431999 | 0.502669993 |
| 0.708536018 | 0.437925992 | 0.498284997 |
| 0.709035976 | 0.563432978 | 0.493602994 |
| 0.704772987 | 0.690152013 | 0.490995990 |
| 0.771151997 | 0.249527010 | 0.504503002 |
| 0.771125969 | 0.375181990 | 0.499646015 |
| 0.771070011 | 0.500524995 | 0.495620983 |
| 0.770958999 | 0.627636003 | 0.491922001 |
| 0.833648065 | 0.312420021 | 0.501821999 |

| | | |
|---|---|---|
| 0.833639024 | 0.437922008 | 0.497001996 |
| 0.833038999 | 0.563451989 | 0.494450989 |
| 0.837284953 | 0.687972035 | 0.489672019 |
| 0.896137995 | 0.249513988 | 0.504312991 |
| 0.896128003 | 0.375144985 | 0.499178992 |
| 0.896076994 | 0.500841035 | 0.495449005 |
| 0.896077945 | 0.624730978 | 0.495480009 |
| 0.958646007 | 0.312412000 | 0.501823011 |
| 0.958545035 | 0.437917997 | 0.497330007 |
| 0.959055033 | 0.563441989 | 0.494504993 |
| 0.954812981 | 0.690138991 | 0.489306993 |
| 0.021138000 | 0.291424989 | 0.502793029 |
| 0.021090999 | 0.417019007 | 0.498680996 |
| 0.021067999 | 0.542325007 | 0.494626985 |
| 0.021075000 | 0.671373029 | 0.491059991 |
| 0.083607001 | 0.354218990 | 0.501486015 |
| 0.083663000 | 0.479780976 | 0.497443994 |
| 0.082526996 | 0.605388978 | 0.491261993 |
| 0.118491007 | 0.730255009 | 0.499875983 |
| 0.146130989 | 0.291426994 | 0.503760991 |
| 0.146080003 | 0.416982002 | 0.500733026 |
| 0.146041009 | 0.542802969 | 0.495311005 |
| 0.145996007 | 0.665454957 | 0.486510990 |
| 0.208609987 | 0.354228990 | 0.503421021 |
| 0.208481988 | 0.479798009 | 0.499778004 |
| 0.209496012 | 0.605321012 | 0.492414998 |
| 0.184129002 | 0.730505996 | 0.499406018 |
| 0.271131988 | 0.291435016 | 0.504956010 |
| 0.271062992 | 0.417044996 | 0.503064980 |
| 0.271051001 | 0.542361985 | 0.498353997 |
| 0.271070986 | 0.671335996 | 0.490943030 |
| 0.333588015 | 0.354240006 | 0.504884004 |
| 0.333630007 | 0.479817019 | 0.502161019 |
| 0.332505994 | 0.605444032 | 0.497931012 |
| 0.368411008 | 0.729843970 | 0.474506001 |
| 0.396134998 | 0.291446005 | 0.505370010 |
| 0.396067001 | 0.417008018 | 0.504187993 |
| 0.396019989 | 0.542846980 | 0.500626030 |
| 0.395976997 | 0.665555011 | 0.497438996 |
| 0.458618980 | 0.354245995 | 0.504823040 |
| 0.458478990 | 0.479815976 | 0.502173010 |
| 0.459496987 | 0.605369967 | 0.498040001 |
| 0.434059994 | 0.730134022 | 0.474925000 |
| 0.521149975 | 0.291449988 | 0.504873975 |
| 0.521081978 | 0.417048018 | 0.502991962 |
| 0.521049003 | 0.542357974 | 0.498528000 |

| | | |
|---|---|---|
| 0.521061993 | 0.671343029 | 0.491560993 |
| 0.583609975 | 0.354243001 | 0.503296024 |
| 0.583639048 | 0.479799987 | 0.499406018 |
| 0.582508992 | 0.605387989 | 0.492554011 |
| 0.618372013 | 0.730245010 | 0.499435978 |
| 0.646150010 | 0.291451994 | 0.503876971 |
| 0.646081966 | 0.416989008 | 0.500230000 |
| 0.646020013 | 0.542801046 | 0.495099987 |
| 0.645958012 | 0.665439024 | 0.486411017 |
| 0.708630043 | 0.354232012 | 0.501153006 |
| 0.708482011 | 0.479777020 | 0.496781993 |
| 0.709498010 | 0.605312990 | 0.491179990 |
| 0.684025996 | 0.730503963 | 0.499116983 |
| 0.771149998 | 0.291441994 | 0.502977029 |
| 0.771094040 | 0.417019007 | 0.498026999 |
| 0.771053024 | 0.542319018 | 0.494491990 |
| 0.771058020 | 0.671361051 | 0.490427001 |
| 0.833623036 | 0.354218990 | 0.499991015 |
| 0.833665005 | 0.479773998 | 0.495812007 |
| 0.832523957 | 0.605400956 | 0.494246994 |
| 0.868403965 | 0.730118967 | 0.478341022 |
| 0.896143991 | 0.291431994 | 0.502565971 |
| 0.896098977 | 0.416965986 | 0.497563993 |
| 0.896043019 | 0.542801046 | 0.494866001 |
| 0.895980970 | 0.665503034 | 0.495362985 |
| 0.958632018 | 0.354214017 | 0.500222977 |
| 0.958498023 | 0.479770976 | 0.496034003 |
| 0.959502983 | 0.605337000 | 0.494336020 |
| 0.934042959 | 0.730394019 | 0.478718988 |
| 0.083613002 | 0.230605995 | 0.505094991 |
| 0.208617005 | 0.230611984 | 0.505248018 |
| 0.333622989 | 0.230618989 | 0.505415029 |
| 0.458637014 | 0.230634017 | 0.505442965 |
| 0.583648993 | 0.230638000 | 0.505339987 |
| 0.708649980 | 0.230635006 | 0.505219988 |
| 0.833641023 | 0.230627011 | 0.505129981 |
| 0.958628972 | 0.230617011 | 0.505066992 |
| 0.833661008 | 0.759446030 | 0.467757985 |
| 0.583587991 | 0.759670039 | 0.508022002 |
| 0.333602005 | 0.758898948 | 0.460888008 |
| 0.083750001 | 0.759678994 | 0.508907961 |
| 0.934365003 | 0.813187019 | 0.559882987 |
| 0.818271993 | 0.838685000 | 0.545724983 |
| 0.840022992 | 0.880186005 | 0.608983971 |
| 0.875822014 | 0.872753993 | 0.502546008 |
| 0.017676000 | 0.845332020 | 0.659536012 |

```
0.996180011      0.876573954      0.570818016
0.961513949      0.884266018      0.677816996
0.899605011      0.820959962      0.665833014
0.917497003      0.835936017      0.605726007
0.859627984      0.858008045      0.563600002
0.976402958      0.861839983      0.629976993
```

IM15'
E+ZPE = -1200.55598 eV
1.0
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    20.0422000885       0.0000000000        0.0000000000
     0.0000000000      34.7140998840        0.0000000000
     0.0000000000       0.0000000000       15.0721998215
```
  B   N   O
 64   64   14
Direct
```
  0.032549001      0.251850998      0.486817013
  0.032568001      0.377483999      0.494659001
  0.032590003      0.502782005      0.503459997
  0.032575998      0.629904991      0.513765991
  0.095050996      0.314729009      0.491287998
  0.095138996      0.440200007      0.500172010
  0.094573997      0.565664988      0.509824987
  0.099161998      0.690283000      0.517930984
  0.157542003      0.251848003      0.487114020
  0.157570006      0.377427983      0.496384001
  0.157610000      0.503085023      0.506290959
  0.157719001      0.626869033      0.513896999
  0.220061007      0.314707993      0.491970975
  0.220046993      0.440162974      0.501920990
  0.220647019      0.565648999      0.512328032
  0.216891006      0.692080949      0.517888022
  0.282539993      0.251835998      0.487129016
  0.282566996      0.377433011      0.496895000
  0.282611986      0.502735027      0.507700983
  0.282621003      0.629964990      0.517499995
  0.345074009      0.314704009      0.491682004
  0.345139008      0.440145996      0.501739964
  0.344610000      0.565617956      0.513882984
  0.348412002      0.691906995      0.515383015
  0.407554993      0.251823992      0.486824986
  0.407579023      0.377409989      0.495723012
  0.407604004      0.503023980      0.506327974
  0.407564986      0.626770023      0.521243997
  0.470073997      0.314704009      0.490456012
```

| | | |
|---|---|---|
| 0.470043972 | 0.440175007 | 0.499099994 |
| 0.470579998 | 0.565549000 | 0.509854029 |
| 0.465876006 | 0.690105969 | 0.515568976 |
| 0.532567972 | 0.251825998 | 0.486317024 |
| 0.532568971 | 0.377459000 | 0.493298996 |
| 0.532587005 | 0.502775027 | 0.501281989 |
| 0.532551984 | 0.629470985 | 0.511044018 |
| 0.595063992 | 0.314718020 | 0.489061997 |
| 0.595109006 | 0.440213001 | 0.495406011 |
| 0.594596011 | 0.565687021 | 0.501748981 |
| 0.599093966 | 0.689948004 | 0.519001006 |
| 0.657575002 | 0.251830009 | 0.485989994 |
| 0.657560013 | 0.377458011 | 0.491313023 |
| 0.657562012 | 0.503130957 | 0.496916007 |
| 0.657599983 | 0.627166997 | 0.500501982 |
| 0.720067026 | 0.314734009 | 0.488445995 |
| 0.720013970 | 0.440232012 | 0.493666996 |
| 0.720536007 | 0.565778009 | 0.499267986 |
| 0.716413008 | 0.691950016 | 0.520192989 |
| 0.782577988 | 0.251843992 | 0.486042005 |
| 0.782563998 | 0.377496994 | 0.491136995 |
| 0.782567995 | 0.502851015 | 0.497092983 |
| 0.782530024 | 0.629844003 | 0.507175020 |
| 0.845065015 | 0.314738981 | 0.488902009 |
| 0.845116025 | 0.440241984 | 0.494777007 |
| 0.844582045 | 0.565711966 | 0.503206017 |
| 0.848855026 | 0.690067014 | 0.517072961 |
| 0.907565033 | 0.251846987 | 0.486393997 |
| 0.907565985 | 0.377473999 | 0.492572012 |
| 0.907581973 | 0.503127001 | 0.500108008 |
| 0.907658011 | 0.626856011 | 0.513031003 |
| 0.970062006 | 0.314738981 | 0.490056976 |
| 0.970030981 | 0.440221023 | 0.497407992 |
| 0.970613021 | 0.565680977 | 0.507170021 |
| 0.966415982 | 0.692390012 | 0.517449978 |
| 0.032554000 | 0.293754992 | 0.489405004 |
| 0.032578000 | 0.419310000 | 0.497414003 |
| 0.032574003 | 0.544541028 | 0.506820971 |
| 0.032690998 | 0.673657016 | 0.516789020 |
| 0.095050996 | 0.356513994 | 0.494181000 |
| 0.095174998 | 0.482026008 | 0.503377963 |
| 0.094052002 | 0.607579010 | 0.512607987 |
| 0.130802000 | 0.732602018 | 0.523756976 |
| 0.157547998 | 0.293745020 | 0.490224019 |
| 0.157583995 | 0.419227996 | 0.499632000 |
| 0.157588004 | 0.545003991 | 0.509655002 |

| | | |
|---|---|---|
| 0.157573004 | 0.667589002 | 0.515129983 |
| 0.220065004 | 0.356483994 | 0.495229983 |
| 0.220024011 | 0.481983975 | 0.505522025 |
| 0.221159991 | 0.607475001 | 0.514821998 |
| 0.196417999 | 0.732619985 | 0.523298020 |
| 0.282564998 | 0.293729993 | 0.490376002 |
| 0.282588980 | 0.419248023 | 0.500397011 |
| 0.282649006 | 0.544466963 | 0.511638001 |
| 0.282723997 | 0.673293998 | 0.517294989 |
| 0.345068989 | 0.356481989 | 0.494913994 |
| 0.345203007 | 0.481961009 | 0.505615006 |
| 0.344208992 | 0.607440990 | 0.518681000 |
| 0.369206006 | 0.731890982 | 0.498614021 |
| 0.407568983 | 0.293726998 | 0.489709002 |
| 0.407601006 | 0.419214012 | 0.499038018 |
| 0.407649018 | 0.544938991 | 0.510729010 |
| 0.407885983 | 0.667572958 | 0.524909982 |
| 0.470082038 | 0.356494983 | 0.493160996 |
| 0.470039023 | 0.482013975 | 0.502421011 |
| 0.471123019 | 0.607452968 | 0.514862999 |
| 0.434648980 | 0.731507030 | 0.495956998 |
| 0.532574015 | 0.293734004 | 0.488543975 |
| 0.532579011 | 0.419295001 | 0.495832001 |
| 0.532614984 | 0.544586028 | 0.504120006 |
| 0.532568971 | 0.673423008 | 0.515498995 |
| 0.595059995 | 0.356516988 | 0.491019022 |
| 0.595148025 | 0.482070018 | 0.497493000 |
| 0.594126982 | 0.607678020 | 0.503231991 |
| 0.630139985 | 0.730143033 | 0.549674972 |
| 0.657569007 | 0.293747987 | 0.487704997 |
| 0.657557016 | 0.419282995 | 0.493101012 |
| 0.657544025 | 0.545107012 | 0.498314008 |
| 0.657397992 | 0.668038997 | 0.504069988 |
| 0.720068977 | 0.356537016 | 0.490044005 |
| 0.719982994 | 0.482093974 | 0.495373014 |
| 0.720967017 | 0.607714009 | 0.500903011 |
| 0.695674011 | 0.730676983 | 0.547732026 |
| 0.782569994 | 0.293758014 | 0.487685002 |
| 0.782564998 | 0.419339011 | 0.492868007 |
| 0.782545964 | 0.544655972 | 0.499393996 |
| 0.782586981 | 0.673425975 | 0.514482028 |
| 0.845063017 | 0.356540999 | 0.490709993 |
| 0.845144004 | 0.482092985 | 0.497034012 |
| 0.844055012 | 0.607614999 | 0.507693991 |
| 0.879707001 | 0.732463998 | 0.514015986 |
| 0.907567032 | 0.293759992 | 0.488383006 |

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0.907571029        0.419290990        0.494752994
0.907558943        0.545064979        0.503436997
0.907547998        0.667545980        0.518398989
0.970068953        0.356534983        0.492387000
0.969991012        0.482052986        0.500216017
0.971070962        0.607530000        0.511488959
0.945308975        0.732876027        0.514930006
0.095040998        0.232958993        0.485695012
0.220038000        0.232953004        0.485692006
0.345039987        0.232944982        0.485621013
0.470065004        0.232933993        0.485413001
0.595071035        0.232936988        0.485217010
0.720083014        0.232945998        0.485209987
0.845071963        0.232948004        0.485392974
0.970058960        0.232950998        0.485588016
0.844594987        0.761945015        0.509050010
0.469489008        0.759798004        0.475048985
0.595325986        0.757080010        0.578307981
0.096270003        0.762287979        0.529183996
0.316701006        0.829857014        0.511112987
0.255715018        0.829436029        0.499633993
```

TS15
E+ZPE = -1244.05239 eV
1.0
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| 0.264681023 | 0.504362977 | 0.503617992 |
| 0.264598014 | 0.631340031 | 0.489234006 |
| 0.327156987 | 0.316305009 | 0.510433016 |
| 0.327219012 | 0.441789001 | 0.506811987 |
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| 0.330924016 | 0.691528043 | 0.476729978 |
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| 0.389678013 | 0.379037005 | 0.508660972 |
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| 0.577177995 | 0.316320009 | 0.508330999 |
| 0.577225959 | 0.441810018 | 0.501954019 |
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| 0.397914923 | 0.543794168 | 0.506052670 |
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E+ZPE = -1246.30425 eV
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   B   N   O   H   C
  64  64  12   8   3
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Direct
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| 0.022792000 | 0.629450985 | 0.496847987 |
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| 0.085059999 | 0.440018003 | 0.504333966 |
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| 0.147524002 | 0.251605011 | 0.501240007 |
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| 0.147580995 | 0.502822993 | 0.505408987 |
| 0.147958997 | 0.626415027 | 0.498156994 |
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| 0.210017002 | 0.439935009 | 0.507134018 |
| 0.210682002 | 0.565321970 | 0.504221971 |
| 0.206175006 | 0.692071004 | 0.492086006 |
| 0.272546997 | 0.251583006 | 0.502013022 |
| 0.272540002 | 0.377209002 | 0.507058976 |
| 0.272625010 | 0.502502007 | 0.507533022 |
| 0.272516020 | 0.629643016 | 0.500184000 |
| 0.335049989 | 0.314467995 | 0.505136024 |
| 0.335129001 | 0.439933993 | 0.508403005 |
| 0.334563996 | 0.565484001 | 0.505733011 |
| 0.338856011 | 0.690011025 | 0.493086016 |
| 0.397556002 | 0.251596000 | 0.502081990 |
| 0.397557001 | 0.377193013 | 0.507053028 |
| 0.397582006 | 0.502874037 | 0.507457980 |
| 0.397588026 | 0.626779034 | 0.502669993 |
| 0.460079026 | 0.314487006 | 0.504315015 |
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| 0.456305003 | 0.692098037 | 0.492434993 |
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| 0.522571050 | 0.377261996 | 0.504957022 |
| 0.522557013 | 0.502586018 | 0.504472978 |
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| 0.585129976 | 0.440025998 | 0.503745963 |
| 0.584446014 | 0.565472023 | 0.499466982 |
| 0.588726989 | 0.689984981 | 0.492597005 |
| 0.647557001 | 0.251625011 | 0.500481007 |
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| 0.647557001 | 0.502977003 | 0.500985014 |
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| 0.710069010 | 0.314541016 | 0.500540010 |

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| 0.397531996 | 0.544833003 | 0.506466987 |

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| 0.897478988 | 0.545048990 | 0.500233006 |
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0.802366033      0.829879980      0.381183006
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 0.2842551180965103 0.3794967137357688 0.4949645634534150
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 0.3467735566119501 0.3168786535632293 0.4918745075358970
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| 0.275095987 | 0.378596982 | 0.506461988 |
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| 0.735185006 | 0.786965034 | 0.644254014 |
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Direct
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     0.462933978         0.565617956         0.503417003
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| 0.587536978 | 0.440111986 | 0.502158995 |
| 0.586929006 | 0.565888008 | 0.500405015 |
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| 0.272523990 | 0.629557028 | 0.498807005 |
| 0.335254002 | 0.314427995 | 0.506209020 |
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| 0.460265981 | 0.314487006 | 0.505815014 |
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| 0.154970006 | 0.419351017 | 0.501449000 |
| 0.592414982 | 0.356489983 | 0.502648006 |
| 0.655089012 | 0.544885970 | 0.499612986 |
| 0.029994999 | 0.544757015 | 0.503265019 |
| 0.654947975 | 0.293704993 | 0.503997982 |
| 0.154978012 | 0.293764003 | 0.502269977 |
| 0.654945025 | 0.419196980 | 0.503313013 |
| 0.779978987 | 0.293689993 | 0.505345998 |
| 0.092471005 | 0.356552015 | 0.503146002 |
| 0.030001000 | 0.293734004 | 0.503997982 |
| 0.717460983 | 0.356461989 | 0.505087018 |
| 0.904996962 | 0.293709993 | 0.505293006 |
| 0.968238994 | 0.607659999 | 0.502937008 |
| 0.717436002 | 0.481938976 | 0.503929014 |
| 0.030014999 | 0.419357005 | 0.504832974 |
| 0.967513063 | 0.356514983 | 0.505580015 |
| 0.842489997 | 0.356476989 | 0.506329999 |
| 0.904474973 | 0.667702022 | 0.500424978 |
| 0.780000971 | 0.419236018 | 0.506124011 |
| 0.967476043 | 0.482116996 | 0.505976014 |
| 0.780065018 | 0.544444985 | 0.503862988 |
| 0.905041024 | 0.419254012 | 0.506856025 |
| 0.841369981 | 0.607584010 | 0.502907997 |
| 0.842639979 | 0.482000019 | 0.506599007 |
| 0.904978024 | 0.545081023 | 0.505694984 |
| 0.191131993 | 0.730817971 | 0.492943998 |
| 0.120941000 | 0.732083013 | 0.494935982 |
| 0.842121036 | 0.761625019 | 0.471553997 |
| 0.354959990 | 0.767189962 | 0.488550017 |

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| 0.590655969 | 0.761385955 | 0.493234994 |
| 0.467442973 | 0.232922015 | 0.502806000 |
| 0.342460995 | 0.232930999 | 0.502433002 |
| 0.592452002 | 0.232890999 | 0.503500999 |
| 0.217490009 | 0.232938993 | 0.502542022 |
| 0.717476019 | 0.232885999 | 0.504131015 |
| 0.092511998 | 0.232925999 | 0.503039006 |
| 0.842507983 | 0.232893005 | 0.504167018 |
| 0.967518963 | 0.232905010 | 0.503688985 |
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IM19
E+ZPE = -1198.46416 eV
1.0

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B    N    O    H
64   64   12   2
Direct

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| 0.022608000 | 0.502498985 | 0.495953993 |
| 0.022814000 | 0.629678015 | 0.490155019 |
| 0.085087003 | 0.314431017 | 0.501826997 |
| 0.085121001 | 0.439900010 | 0.500379041 |
| 0.084652002 | 0.565379991 | 0.494172015 |
| 0.089107995 | 0.689746028 | 0.488909001 |
| 0.147604002 | 0.251545012 | 0.502090975 |
| 0.147591000 | 0.377155019 | 0.503427032 |
| 0.147571990 | 0.502785961 | 0.500258979 |
| 0.147841002 | 0.626512004 | 0.490872005 |
| 0.210106006 | 0.314435001 | 0.504227982 |
| 0.210025995 | 0.439908004 | 0.505200974 |
| 0.210598018 | 0.565325981 | 0.499122994 |
| 0.206340001 | 0.691964961 | 0.489508013 |
| 0.272619014 | 0.251548995 | 0.502965988 |
| 0.272594985 | 0.377189002 | 0.507071029 |
| 0.272549995 | 0.502492997 | 0.505843993 |
| 0.272430989 | 0.629524006 | 0.496512004 |
| 0.335101997 | 0.314445001 | 0.506143974 |
| 0.335116011 | 0.439933993 | 0.509118978 |
| 0.334450011 | 0.565423013 | 0.504954998 |
| 0.338609006 | 0.689773006 | 0.489472010 |
| 0.397612008 | 0.251567017 | 0.503412004 |

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| 0.397622999 | 0.377196008 | 0.508880974 |
| 0.397528998 | 0.502894970 | 0.509007996 |
| 0.397329981 | 0.626704969 | 0.503032014 |
| 0.460127990 | 0.314464012 | 0.506374006 |
| 0.460053998 | 0.440008003 | 0.509528992 |
| 0.460453983 | 0.565536968 | 0.506195004 |
| 0.455859005 | 0.691756996 | 0.489934004 |
| 0.522602979 | 0.251569984 | 0.503177986 |
| 0.522616968 | 0.377247985 | 0.507567000 |
| 0.522570003 | 0.502668050 | 0.507264014 |
| 0.522086985 | 0.629831036 | 0.499428005 |
| 0.585087008 | 0.314476017 | 0.504732021 |
| 0.585117985 | 0.440023992 | 0.506110028 |
| 0.584480987 | 0.565666966 | 0.502157982 |
| 0.587737970 | 0.690617008 | 0.492255991 |
| 0.647560998 | 0.251573006 | 0.502456002 |
| 0.647583029 | 0.377239991 | 0.504020982 |
| 0.647494953 | 0.502977003 | 0.502280006 |
| 0.647355962 | 0.627040020 | 0.495275003 |
| 0.710071009 | 0.314477006 | 0.502282030 |
| 0.709993020 | 0.440030997 | 0.501209984 |
| 0.710417986 | 0.565569989 | 0.497135029 |
| 0.707356000 | 0.690992993 | 0.491598008 |
| 0.772553992 | 0.251558995 | 0.501651001 |
| 0.772546997 | 0.377247985 | 0.500466992 |
| 0.772499033 | 0.502641017 | 0.497251009 |
| 0.772628031 | 0.629449007 | 0.492663000 |
| 0.835057007 | 0.314462995 | 0.500469997 |
| 0.835065001 | 0.439995998 | 0.497611986 |
| 0.834616005 | 0.565482957 | 0.493356005 |
| 0.838821989 | 0.690186023 | 0.490928002 |
| 0.897541989 | 0.251554023 | 0.501204004 |
| 0.897547033 | 0.377198013 | 0.498841996 |
| 0.897571966 | 0.502869037 | 0.494735974 |
| 0.897978042 | 0.626805023 | 0.490498975 |
| 0.960057995 | 0.314440990 | 0.500298968 |
| 0.960020023 | 0.439935009 | 0.497272997 |
| 0.960705984 | 0.565446034 | 0.492184998 |
| 0.956647984 | 0.692100015 | 0.490126988 |
| 0.022569001 | 0.293431012 | 0.501031995 |
| 0.022561001 | 0.418987009 | 0.499047983 |
| 0.022658000 | 0.544230977 | 0.493796991 |
| 0.023272000 | 0.673318998 | 0.489607005 |
| 0.085077004 | 0.356207019 | 0.501711017 |
| 0.085161001 | 0.481701011 | 0.498784986 |
| 0.084290000 | 0.607235003 | 0.491349026 |

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| 0.147600992 | 0.293433018 | 0.502733995 |
| 0.147578997 | 0.418938988 | 0.503226992 |
| 0.147599993 | 0.544673994 | 0.497707023 |
| 0.147931993 | 0.667162028 | 0.487437001 |
| 0.210104008 | 0.356208008 | 0.505125995 |
| 0.209977008 | 0.481716011 | 0.504122980 |
| 0.211168994 | 0.607111982 | 0.495332993 |
| 0.185335001 | 0.732496965 | 0.492204012 |
| 0.272612995 | 0.293434996 | 0.504656978 |
| 0.272579020 | 0.418994015 | 0.507724995 |
| 0.272546997 | 0.544225977 | 0.503855996 |
| 0.272512999 | 0.673158011 | 0.491205015 |
| 0.335110015 | 0.356221991 | 0.507842020 |
| 0.335139992 | 0.481754967 | 0.508808969 |
| 0.333889003 | 0.607305002 | 0.502378997 |
| 0.369673012 | 0.731494997 | 0.473085000 |
| 0.397621001 | 0.293454995 | 0.505612000 |
| 0.397612983 | 0.418998987 | 0.509975009 |
| 0.397486007 | 0.544812015 | 0.507746983 |
| 0.397044981 | 0.667395982 | 0.498946018 |
| 0.460139029 | 0.356243997 | 0.508153010 |
| 0.460009031 | 0.481846999 | 0.509473027 |
| 0.460801008 | 0.607360002 | 0.504000007 |
| 0.435312006 | 0.731756972 | 0.474203996 |
| 0.522612971 | 0.293457001 | 0.505009002 |
| 0.522602027 | 0.419072008 | 0.508298983 |
| 0.522561010 | 0.544456029 | 0.505837033 |
| 0.521676008 | 0.673215977 | 0.494087007 |
| 0.585098048 | 0.356263996 | 0.505723014 |
| 0.585130975 | 0.481869031 | 0.505666985 |
| 0.583918981 | 0.607629010 | 0.499170007 |
| 0.613479021 | 0.731585051 | 0.492513009 |
| 0.647575035 | 0.293469006 | 0.503228004 |
| 0.647564995 | 0.419048987 | 0.503919017 |
| 0.647432047 | 0.544924980 | 0.500724959 |
| 0.647196986 | 0.667943009 | 0.492122009 |
| 0.710065013 | 0.356263996 | 0.502241029 |
| 0.709909035 | 0.481869031 | 0.500181975 |
| 0.710780048 | 0.607454012 | 0.494985019 |
| 0.683695958 | 0.730332042 | 0.491517017 |
| 0.772558988 | 0.293453979 | 0.501324003 |
| 0.772517019 | 0.419070003 | 0.499563981 |
| 0.772469008 | 0.544412019 | 0.495736996 |
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0.831412030        0.763432033        0.492973009
0.584198009        0.763477033        0.494614994
0.334993008        0.760571018        0.458261990
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TS19
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  64  64  12   2
Direct
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    0.031392015        0.631318878        0.507226651
    0.093571768        0.315772570        0.500916299
    0.093562156        0.441263924        0.505031337
    0.093026398        0.566833438        0.507357723
    0.098499329        0.693688680        0.506351575
    0.156082611        0.252868789        0.498693809
    0.156076710        0.378492313        0.502947385
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| 0.155992785 | 0.504113420 | 0.505648319 |
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| 0.218532440 | 0.441227963 | 0.503654248 |
| 0.218931046 | 0.566539595 | 0.503253156 |
| 0.215027953 | 0.691604965 | 0.496955173 |
| 0.281093055 | 0.252854641 | 0.498441157 |
| 0.281107806 | 0.378504374 | 0.501502466 |
| 0.281090867 | 0.503778917 | 0.501872776 |
| 0.280746839 | 0.630272735 | 0.497866505 |
| 0.343605992 | 0.315760592 | 0.499475018 |
| 0.343675345 | 0.441236150 | 0.500804241 |
| 0.343133323 | 0.566588330 | 0.497614137 |
| 0.345616673 | 0.691367879 | 0.497580602 |
| 0.406109079 | 0.252870548 | 0.497926551 |
| 0.406130777 | 0.378502588 | 0.499581476 |
| 0.406167369 | 0.504134079 | 0.498556378 |
| 0.406009344 | 0.627932264 | 0.492380767 |
| 0.468620850 | 0.315785674 | 0.498316065 |
| 0.468616139 | 0.441285847 | 0.498822444 |
| 0.469121046 | 0.566836899 | 0.496793192 |
| 0.464004079 | 0.691884522 | 0.501183155 |
| 0.531118346 | 0.252899064 | 0.497467247 |
| 0.531140520 | 0.378574620 | 0.498373201 |
| 0.531137046 | 0.503968036 | 0.498213529 |
| 0.530944667 | 0.631331240 | 0.498917956 |
| 0.593619648 | 0.315821937 | 0.497734800 |
| 0.593683886 | 0.441374665 | 0.498505981 |
| 0.593035230 | 0.567029370 | 0.499237868 |
| 0.596946912 | 0.693734119 | 0.503099843 |
| 0.656121808 | 0.252923734 | 0.497341997 |
| 0.656129754 | 0.378595884 | 0.498366778 |
| 0.656100633 | 0.504394625 | 0.499430884 |
| 0.655948319 | 0.628324678 | 0.502721435 |
| 0.718611500 | 0.315846717 | 0.498036869 |
| 0.718550165 | 0.441432247 | 0.499575433 |
| 0.719086476 | 0.567065139 | 0.501523189 |
| 0.714649808 | 0.691722491 | 0.503781903 |
| 0.781105570 | 0.252928541 | 0.497566524 |
| 0.781099669 | 0.378645691 | 0.499498651 |
| 0.781070073 | 0.504094574 | 0.501569631 |
| 0.781161480 | 0.631339537 | 0.503622896 |
| 0.843588029 | 0.315844217 | 0.498997396 |
| 0.843612392 | 0.441428401 | 0.501707315 |
| 0.843069181 | 0.567051458 | 0.503892062 |
| 0.847552671 | 0.693866590 | 0.504840978 |

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| 0.906080053 | 0.252916152 | 0.498018805 |
| 0.906066730 | 0.378586818 | 0.501270537 |
| 0.906048839 | 0.504383197 | 0.504321817 |
| 0.906121831 | 0.628314183 | 0.504949271 |
| 0.968574266 | 0.315808970 | 0.500188239 |
| 0.968481859 | 0.441359171 | 0.504005480 |
| 0.969126899 | 0.567028656 | 0.506438260 |
| 0.965189284 | 0.691603262 | 0.506017205 |
| 0.031062504 | 0.294790339 | 0.499986618 |
| 0.031000765 | 0.420374935 | 0.504233361 |
| 0.030985377 | 0.545740796 | 0.507176507 |
| 0.031522599 | 0.675248539 | 0.506401467 |
| 0.093556523 | 0.357558626 | 0.502438190 |
| 0.093545704 | 0.483085283 | 0.506202945 |
| 0.092549274 | 0.608717625 | 0.508291137 |
| 0.125140989 | 0.734081399 | 0.492402185 |
| 0.156083372 | 0.294771246 | 0.500200040 |
| 0.156046745 | 0.420287903 | 0.504258322 |
| 0.155927454 | 0.545996673 | 0.506092849 |
| 0.156224373 | 0.668695529 | 0.507159486 |
| 0.218601650 | 0.357538846 | 0.501867366 |
| 0.218476910 | 0.483040778 | 0.504121651 |
| 0.219308548 | 0.608287685 | 0.502716436 |
| 0.188018486 | 0.731772796 | 0.479232233 |
| 0.281104261 | 0.294757537 | 0.499563158 |
| 0.281110447 | 0.420319413 | 0.502174686 |
| 0.281093412 | 0.545504425 | 0.500888173 |
| 0.280471022 | 0.673388942 | 0.496245020 |
| 0.343620291 | 0.357548296 | 0.500237878 |
| 0.343739202 | 0.483055448 | 0.500331997 |
| 0.342725344 | 0.608378947 | 0.494909375 |
| 0.365303127 | 0.731093023 | 0.511276423 |
| 0.406120023 | 0.294777345 | 0.498541287 |
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| 0.406231654 | 0.546059200 | 0.497098298 |
| 0.406042129 | 0.668836297 | 0.490686392 |
| 0.468653968 | 0.357579560 | 0.498694315 |
| 0.468616805 | 0.483124183 | 0.498336977 |
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| 0.433226572 | 0.733260089 | 0.515578341 |
| 0.531126958 | 0.294806657 | 0.497717938 |
| 0.531172210 | 0.420406335 | 0.498459348 |
| 0.531134239 | 0.545780796 | 0.497983624 |
| 0.530589267 | 0.675165133 | 0.501823359 |
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0.968565320        0.233992004        0.497701550
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Direct
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    0.095650998       0.314402996       0.504154015
    0.095686002       0.439940998       0.501124026
    0.095141000       0.565451034       0.497139996
    0.099143001       0.691682986       0.495424012
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    0.158140006       0.377149992       0.503072035
    0.158139007       0.502841015       0.499428986
    0.158167997       0.626613047       0.495970001
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    0.408147025       0.251466002       0.504568996
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    0.408139982       0.502820026       0.500451996
    0.408060994       0.626727002       0.498490004
    0.470635004       0.314368985       0.503296973
    0.470583995       0.439883004       0.501380032
    0.471118022       0.565442024       0.499211008
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    0.595035014       0.565374002       0.498272975
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| 0.094764003 | 0.607307035 | 0.495997019 |
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| 0.158420998 | 0.667404003 | 0.495304994 |
| 0.220641000 | 0.356198997 | 0.503629982 |
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| 0.283141993 | 0.418998987 | 0.502187025 |
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| 0.283143016 | 0.673425041 | 0.496495996 |
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| 0.533025009 | 0.673477018 | 0.495556001 |
| 0.595615007 | 0.356177981 | 0.501999007 |
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| 0.908159063 | 0.293406012 | 0.503525011 |
| 0.908138983 | 0.418982009 | 0.500888996 |
| 0.908136033 | 0.544839981 | 0.497184003 |
| 0.907998993 | 0.667536035 | 0.494069005 |
| 0.970646043 | 0.356207019 | 0.502705996 |
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| 0.971664041 | 0.607442034 | 0.495496998 |
| 0.939513994 | 0.731233021 | 0.494195015 |
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| 0.220650992 | 0.232571002 | 0.505186010 |
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Direct
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  0.096652002      0.316933986      0.488658026
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  0.159139006      0.254047019      0.484941010
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  0.284176002      0.379631010      0.495501997
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  0.350419994      0.692321991      0.516047009
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| 0.471653002 | 0.442339985 | 0.501136017 |
| 0.472198021 | 0.567806999 | 0.511048005 |
| 0.467880025 | 0.694598011 | 0.516830971 |
| 0.534152972 | 0.254026003 | 0.486104013 |
| 0.534184995 | 0.379634005 | 0.495878982 |
| 0.534194988 | 0.504950004 | 0.505232991 |
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| 0.600521989 | 0.692424022 | 0.518313000 |
| 0.659156005 | 0.254025014 | 0.485894008 |
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| 0.659170994 | 0.505325990 | 0.502767973 |
| 0.659242988 | 0.629181976 | 0.510209027 |
| 0.721656975 | 0.316917997 | 0.489518991 |
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| 0.846640023 | 0.316935003 | 0.488265982 |
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| 0.846146013 | 0.567917987 | 0.505434992 |
| 0.850785006 | 0.692502978 | 0.515823020 |
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| 0.909142040 | 0.379660021 | 0.492038994 |
| 0.909146037 | 0.505319012 | 0.500928985 |
| 0.909292974 | 0.629087966 | 0.510576014 |
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| 0.221603015 | 0.484164008 | 0.503404981 |
| 0.222670000 | 0.609674978 | 0.511017032 |
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| 0.284193989 | 0.546674028 | 0.508795966 |
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| 0.409157028 | 0.295920025 | 0.489477009 |
| 0.409198997 | 0.421395007 | 0.499692996 |
| 0.409191003 | 0.547145013 | 0.510039991 |
| 0.409079991 | 0.669777001 | 0.518854022 |
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| 0.471626973 | 0.484168019 | 0.504566022 |
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| 0.446813988 | 0.735090015 | 0.512461002 |
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| 0.534172005 | 0.675827049 | 0.516960966 |
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| 0.270961997 | 0.671364018 | 0.489300982 |
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| 0.332563998 | 0.605409033 | 0.497628975 |
| 0.368045996 | 0.729933035 | 0.475899985 |
| 0.396147988 | 0.291414000 | 0.504701966 |
| 0.396093005 | 0.416992991 | 0.503399002 |
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| 0.459521017 | 0.605411011 | 0.497535994 |
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| 0.708480013 | 0.479824986 | 0.497720975 |
| 0.709545023 | 0.605395022 | 0.491457983 |
| 0.684156993 | 0.730739016 | 0.495230996 |
| 0.771132012 | 0.291456994 | 0.503014013 |
| 0.771085999 | 0.417042991 | 0.499096008 |
| 0.771065015 | 0.542364018 | 0.494641980 |
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| 0.934953989 | 0.813022955 | 0.561119988 |
| 0.819187020 | 0.838822032 | 0.547807005 |
| 0.841477995 | 0.880306992 | 0.610824984 |
| 0.876726001 | 0.872763993 | 0.504104978 |
| 0.019073000 | 0.845076968 | 0.660180962 |
| 0.997544986 | 0.876210990 | 0.571196962 |
| 0.963365987 | 0.884202008 | 0.678329007 |
| 0.900900990 | 0.820999961 | 0.667343991 |
| 0.918613023 | 0.835875963 | 0.607020967 |
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  0.095020002     0.314609999     0.491207008
  0.095058003     0.440073003     0.500406977
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  0.157511990     0.251731988     0.486898984
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  0.282506994     0.251729982     0.487040021
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| 0.845031041 | 0.314652004 | 0.488854997 |
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| 0.157483999 | 0.544884047 | 0.508974018 |
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| 0.407537007 | 0.544861959 | 0.507368036 |
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| 0.532505971 | 0.419200002 | 0.495731997 |
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| 0.595099965 | 0.481971997 | 0.497501985 |
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  0.077747722          0.316419156          0.508113875
  0.077710994          0.441869797          0.504904157
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  0.202729022          0.316427975          0.509726754
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  0.203118277          0.567414915          0.498806784
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| 0.390015117 | 0.628076548 | 0.493820941 |
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| 0.452682771 | 0.441986582 | 0.509470274 |
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| 0.699304332 | 0.693739998 | 0.477521374 |
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| 0.890221867 | 0.379092389 | 0.503864411 |
| 0.890137930 | 0.504668908 | 0.495166931 |
| 0.890370327 | 0.629308678 | 0.485734653 |
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| 0.952624148 | 0.441826364 | 0.501390504 |
| 0.953035554 | 0.567249752 | 0.491488702 |
| 0.950163139 | 0.695375421 | 0.480900160 |
| 0.015244592 | 0.295431651 | 0.507571461 |
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| 0.140236903 | 0.420981769 | 0.507705918 |
| 0.140102159 | 0.546766061 | 0.499606121 |
| 0.139779580 | 0.669056789 | 0.480786520 |
| 0.202745343 | 0.358244168 | 0.509980988 |
| 0.202614418 | 0.483853022 | 0.507065967 |
| 0.203427878 | 0.609226576 | 0.492436068 |
| 0.177884156 | 0.734065355 | 0.468863630 |
| 0.265235630 | 0.295454893 | 0.510007785 |
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| 0.264634843 | 0.674661567 | 0.479361343 |
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| 0.358803460 | 0.732742292 | 0.453798755 |
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| 0.453609361 | 0.609501189 | 0.493649943 |
| 0.420706165 | 0.732810038 | 0.453747440 |
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| 0.515017199 | 0.546459086 | 0.498355864 |
| 0.515273054 | 0.674678764 | 0.478157149 |
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| 0.576638353 | 0.609142236 | 0.483589009 |
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| 0.822381002 | 0.763297749 | 0.455879354 |
| 0.575233265 | 0.762418692 | 0.497810254 |
| 0.077726001 | 0.763416868 | 0.465017694 |
| 0.941322160 | 0.765795580 | 0.548898857 |
| 0.895253707 | 0.786824486 | 0.607050010 |
| 0.984167508 | 0.748559108 | 0.688261527 |
| 0.047192454 | 0.776819863 | 0.634237593 |
| 0.987766806 | 0.798816452 | 0.704755660 |
| 0.927268237 | 0.828208349 | 0.474802091 |
| 0.952051911 | 0.847050409 | 0.579652484 |
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Direct
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| 0.085300997 | 0.438719994 | 0.498272975 |
| 0.084756001 | 0.564255003 | 0.494000986 |
| 0.088867003 | 0.688824004 | 0.496578979 |
| 0.147749012 | 0.250288981 | 0.502120018 |
| 0.147753996 | 0.375947999 | 0.500604992 |
| 0.147747989 | 0.501654983 | 0.497626982 |
| 0.147807004 | 0.625559981 | 0.489475016 |
| 0.210255989 | 0.313199024 | 0.502045988 |
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| 0.210729990 | 0.564275002 | 0.497333993 |
| 0.206532000 | 0.690347011 | 0.500152996 |
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| 0.272756982 | 0.501384986 | 0.501537963 |
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| 0.335242987 | 0.313183997 | 0.502894995 |
| 0.335285003 | 0.438722027 | 0.503029989 |
| 0.334798987 | 0.564311980 | 0.503248980 |
| 0.338355982 | 0.689569986 | 0.497420014 |
| 0.397744004 | 0.250262003 | 0.502746997 |
| 0.397736985 | 0.375921982 | 0.503114997 |
| 0.397729990 | 0.501643005 | 0.503520013 |
| 0.397645007 | 0.625926955 | 0.506696987 |
| 0.460255989 | 0.313169986 | 0.502725010 |
| 0.460187992 | 0.438708017 | 0.502714981 |
| 0.460622999 | 0.564320991 | 0.502906036 |
| 0.457224979 | 0.690178990 | 0.493997000 |
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| 0.522738972 | 0.375935993 | 0.501933993 |
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| 0.437926995 | 0.730195010 | 0.473939006 |
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| 0.522723983 | 0.417782022 | 0.501697001 |
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| 0.523156991 | 0.671745992 | 0.496585022 |
| 0.585228045 | 0.354964999 | 0.501156992 |
| 0.585259022 | 0.480533990 | 0.499319997 |
| 0.584292986 | 0.606014026 | 0.495135009 |
| 0.619869983 | 0.730536985 | 0.508329987 |
| 0.647757993 | 0.292172014 | 0.501242981 |
| 0.647710981 | 0.417717022 | 0.498997997 |
| 0.647703986 | 0.543479006 | 0.495718994 |
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IM@N2
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0.9719488504218228 0.3581953962839487 0.4916135359174638
0.9720865698987753 0.4838777076548825 0.4986959811826954
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0.3467065871712980 0.2345352687160253 0.4856120155259518
0.4717290423025303 0.2344351448771703 0.4858608073120146
0.5968362438160535 0.2343841147427983 0.4859684732495052
0.7219375106173824 0.2344004172535185 0.4858987529732733
0.8469766863603292 0.2344837690129751 0.4857149904781070
0.9719490524564859 0.2345680814725585 0.4854889199681726
0.8470228010936580 0.7635429140054352 0.5302703978784613

0.3454679338625698  0.7624686293922094  0.5251414348320548
0.5967936768725830  0.7634696718174288  0.5228008853814283


IM23
E+ZPE = -1239.62153 eV
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       0.0000000000        0.0000000000       15.0721998215
    B   N   O   H   C
   64  64  11   8   3
Direct
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    0.022670001        0.377346995        0.502355997
    0.022606000        0.502751016        0.501420021
    0.023046000        0.629661038        0.494440991
    0.085173003        0.314545989        0.502484981
    0.085189997        0.440060997        0.503745014
    0.084763995        0.565441035        0.499635005
    0.089240996        0.690406955        0.488678020
    0.147677006        0.251621989        0.501685011
    0.147666003        0.377258974        0.504728035
    0.147694006        0.502852993        0.503966978
    0.147992995        0.626484971        0.494890013
    0.210192988        0.314504011        0.504235986
    0.210144001        0.439965009        0.506446011
    0.210788993        0.565307025        0.502219010
    0.206112005        0.691218046        0.489827008
    0.272699002        0.251591000        0.502416013
    0.272691008        0.377234002        0.506719006
    0.272747989        0.502508985        0.506596033
    0.272671998        0.629441974        0.498243996
    0.335204991        0.314476017        0.505218976
    0.335256001        0.439942976        0.507959013
    0.334739008        0.565428947        0.504845028
    0.338942994        0.689848994        0.490908008
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    0.397713003        0.377200019        0.507029996
    0.397719998        0.502860026        0.507124021
    0.397738984        0.626742001        0.502208000
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    0.460169006        0.439975998        0.506952992
    0.460687998        0.565473012        0.503714991
    0.456305003        0.692076993        0.490487997
    0.522741018        0.251606989        0.502304018

| 0.522728028 | 0.377266996 | 0.505384974 |
| 0.522690009 | 0.502587007 | 0.504404010 |
| 0.522478977 | 0.629659005 | 0.496872000 |
| 0.585225999 | 0.314527994 | 0.503338986 |
| 0.585259022 | 0.440039019 | 0.503997982 |
| 0.584586004 | 0.565482957 | 0.499011000 |
| 0.588763010 | 0.689989981 | 0.491453997 |
| 0.647736010 | 0.251645011 | 0.501577034 |
| 0.647726017 | 0.377299990 | 0.502891008 |
| 0.647678957 | 0.502991013 | 0.500706957 |
| 0.647494953 | 0.626633981 | 0.491094001 |
| 0.710221990 | 0.314568983 | 0.501664985 |
| 0.710181021 | 0.440133991 | 0.501286988 |
| 0.710637964 | 0.565650977 | 0.496234011 |
| 0.706453011 | 0.691666997 | 0.490256004 |
| 0.772717012 | 0.251666988 | 0.500864984 |
| 0.772710017 | 0.377374000 | 0.501083025 |
| 0.772726005 | 0.502841015 | 0.499159978 |
| 0.772423994 | 0.630136033 | 0.492528005 |
| 0.835193952 | 0.314589999 | 0.500711988 |
| 0.835242011 | 0.440178001 | 0.500432001 |
| 0.834675008 | 0.565983007 | 0.497225985 |
| 0.838374040 | 0.691769029 | 0.489346001 |
| 0.897689021 | 0.251673994 | 0.500579999 |
| 0.897683977 | 0.377350979 | 0.500904023 |
| 0.897640962 | 0.503186011 | 0.499788001 |
| 0.897674936 | 0.627614960 | 0.496553005 |
| 0.960187040 | 0.314581977 | 0.501048034 |
| 0.960109004 | 0.440150996 | 0.501429006 |
| 0.960595020 | 0.565860975 | 0.498416005 |
| 0.957638002 | 0.691510955 | 0.486692016 |
| 0.022676000 | 0.293544006 | 0.501362979 |
| 0.022650000 | 0.419153986 | 0.502534999 |
| 0.022618999 | 0.544485974 | 0.499927014 |
| 0.024086000 | 0.672828014 | 0.490013001 |
| 0.085156998 | 0.356323007 | 0.503224018 |
| 0.085212997 | 0.481870020 | 0.503233003 |
| 0.084583000 | 0.607190003 | 0.496416998 |
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| 0.147678006 | 0.293514995 | 0.502853993 |
| 0.147661994 | 0.419047998 | 0.505219988 |
| 0.147800997 | 0.544723993 | 0.502142006 |
| 0.148494999 | 0.667109006 | 0.490195988 |
| 0.210182996 | 0.356278007 | 0.505480992 |
| 0.210152995 | 0.481772988 | 0.506086996 |
| 0.211472004 | 0.607144015 | 0.498661982 |

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| 0.272697003 | 0.293479995 | 0.504174010 |
| 0.272701000 | 0.419037009 | 0.507507966 |
| 0.272825978 | 0.544268009 | 0.505104007 |
| 0.272684988 | 0.673338998 | 0.492623011 |
| 0.335195998 | 0.356249986 | 0.506713976 |
| 0.335326995 | 0.481767000 | 0.507882009 |
| 0.334268980 | 0.607383023 | 0.502602986 |
| 0.369673988 | 0.731765983 | 0.476673000 |
| 0.397722996 | 0.293479006 | 0.504472978 |
| 0.397718999 | 0.418992009 | 0.507836989 |
| 0.397715002 | 0.544807949 | 0.506056024 |
| 0.397540014 | 0.667527958 | 0.498933996 |
| 0.460235004 | 0.356265013 | 0.506066970 |
| 0.460125991 | 0.481802988 | 0.506727991 |
| 0.461072994 | 0.607366980 | 0.501780997 |
| 0.435203992 | 0.732236967 | 0.476740988 |
| 0.522736022 | 0.293497001 | 0.503648996 |
| 0.522720985 | 0.419079014 | 0.505752025 |
| 0.522629007 | 0.544350041 | 0.502785025 |
| 0.522380003 | 0.673407953 | 0.493193012 |
| 0.585225000 | 0.356308007 | 0.504003993 |
| 0.585263019 | 0.481857988 | 0.503203992 |
| 0.583875014 | 0.607373024 | 0.495445019 |
| 0.619946021 | 0.732248011 | 0.497747012 |
| 0.647730014 | 0.293537000 | 0.502209012 |
| 0.647723971 | 0.419100992 | 0.502744024 |
| 0.647575987 | 0.544893003 | 0.498481019 |
| 0.647010983 | 0.667361037 | 0.487525995 |
| 0.710227034 | 0.356348996 | 0.501806971 |
| 0.710129964 | 0.481956009 | 0.500294982 |
| 0.710901956 | 0.607419012 | 0.492781005 |
| 0.685447975 | 0.732323010 | 0.496722009 |
| 0.772712016 | 0.293559994 | 0.500944962 |
| 0.772710017 | 0.419187996 | 0.500800001 |
| 0.772701024 | 0.544588995 | 0.497473005 |
| 0.771761016 | 0.673353009 | 0.489814005 |
| 0.835187956 | 0.356368995 | 0.500720023 |
| 0.835263043 | 0.482000019 | 0.499773005 |
| 0.834149022 | 0.607859008 | 0.495756009 |
| 0.863116983 | 0.730780004 | 0.483184025 |
| 0.897689021 | 0.293567989 | 0.500590028 |
| 0.897673033 | 0.419147008 | 0.500823982 |
| 0.897614030 | 0.545108001 | 0.498712000 |
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| 0.960184947 | 0.356361001 | 0.501301003 |

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0.585250981        0.232693996        0.501506990
0.710233981        0.232720012        0.501038006
0.835204991        0.232731001        0.500630966
0.960174003        0.232724984        0.500570001
0.832922991        0.761232990        0.438810000
0.334345994        0.760862993        0.464738024
0.585381977        0.761969960        0.504988026
0.957216985        0.755996010        0.479063988
0.779124010        0.779452034        0.548937011
0.899670010        0.791459988        0.585364014
0.905915034        0.824181028        0.493346008
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0.729465016        0.804180023        0.411558004
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0.803637935        0.830928047        0.386207004
0.812299050        0.792532999        0.499040011
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TS23
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  64  64  11   8   3
Direct
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   0.025158577        0.378630691        0.503025655
   0.025147939        0.503956718        0.496059723
   0.025550819        0.630732071        0.490517925
   0.087679115        0.315866140        0.507333331
   0.087696418        0.441326589        0.501016366
   0.087358011        0.566650912        0.494594304
   0.091991157        0.690555745        0.484660075
   0.150203454        0.252977607        0.510350095
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| 0.212654902 | 0.441273567 | 0.503800568 |
| 0.213417258 | 0.566634099 | 0.496619000 |
| 0.209246580 | 0.693176872 | 0.484859482 |
| 0.275246137 | 0.252968981 | 0.510667571 |
| 0.275210045 | 0.378560032 | 0.507232915 |
| 0.275292721 | 0.503810401 | 0.501110960 |
| 0.275290865 | 0.631053551 | 0.492370042 |
| 0.337749224 | 0.315844300 | 0.509262199 |
| 0.337795118 | 0.441275051 | 0.504696777 |
| 0.337217337 | 0.566785636 | 0.497189507 |
| 0.341455916 | 0.692509022 | 0.486639246 |
| 0.400281979 | 0.252984612 | 0.510544789 |
| 0.400266752 | 0.378560472 | 0.506951822 |
| 0.400235870 | 0.504199627 | 0.500128509 |
| 0.400042873 | 0.628134405 | 0.493980643 |
| 0.462780379 | 0.315871332 | 0.508369216 |
| 0.462727609 | 0.441338924 | 0.502678504 |
| 0.463104945 | 0.566774702 | 0.493637383 |
| 0.458082764 | 0.692634515 | 0.486908475 |
| 0.525291626 | 0.253011865 | 0.510015188 |
| 0.525283347 | 0.378627861 | 0.504637047 |
| 0.525203264 | 0.503938311 | 0.495729181 |
| 0.524689031 | 0.630902398 | 0.486726500 |
| 0.587771754 | 0.315904134 | 0.506668324 |
| 0.587803112 | 0.441386039 | 0.498732248 |
| 0.587042873 | 0.566865361 | 0.486893543 |
| 0.590694226 | 0.691467659 | 0.486560628 |
| 0.650271772 | 0.253038760 | 0.509453665 |
| 0.650261827 | 0.378649345 | 0.501881476 |
| 0.650163044 | 0.504317154 | 0.491122506 |
| 0.649852944 | 0.628249953 | 0.478020667 |
| 0.712752281 | 0.315925068 | 0.505293607 |
| 0.712693611 | 0.441443703 | 0.495917611 |
| 0.713026456 | 0.566986238 | 0.484788869 |
| 0.708950897 | 0.692659460 | 0.488741927 |
| 0.775234931 | 0.253042112 | 0.509224899 |
| 0.775221179 | 0.378687449 | 0.500474205 |
| 0.775206286 | 0.504128859 | 0.490605844 |
| 0.774898374 | 0.631232945 | 0.484301313 |
| 0.837708540 | 0.315924683 | 0.504997960 |
| 0.837735757 | 0.441452851 | 0.495867624 |
| 0.837202349 | 0.567173379 | 0.488488958 |
| 0.840676502 | 0.692385671 | 0.485637844 |

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| 0.900200469 | 0.253030518 | 0.509385108 |
| 0.900178390 | 0.378651295 | 0.501021491 |
| 0.900157548 | 0.504398966 | 0.492981994 |
| 0.900307626 | 0.628734014 | 0.491260790 |
| 0.962688305 | 0.315903859 | 0.505826656 |
| 0.962602655 | 0.441401231 | 0.497905513 |
| 0.963166898 | 0.566997612 | 0.492179462 |
| 0.960009935 | 0.692841711 | 0.485467036 |
| 0.025172585 | 0.294874761 | 0.507655615 |
| 0.025130090 | 0.420421637 | 0.500563611 |
| 0.025189167 | 0.545699698 | 0.494135031 |
| 0.026370072 | 0.674187835 | 0.486855325 |
| 0.087644885 | 0.357625301 | 0.505367036 |
| 0.087741301 | 0.483125227 | 0.498817604 |
| 0.087090028 | 0.608469056 | 0.492341601 |
| 0.121458743 | 0.732671633 | 0.479582136 |
| 0.150190143 | 0.294854624 | 0.508926879 |
| 0.150157037 | 0.420334798 | 0.503653362 |
| 0.150346062 | 0.546000134 | 0.496947106 |
| 0.150959303 | 0.668333060 | 0.487260309 |
| 0.212687496 | 0.357595988 | 0.507441275 |
| 0.212666012 | 0.483056052 | 0.501696590 |
| 0.214068078 | 0.608424661 | 0.493659719 |
| 0.186775919 | 0.733899752 | 0.480063333 |
| 0.275235097 | 0.294846987 | 0.509777247 |
| 0.275215802 | 0.420349550 | 0.505693244 |
| 0.275359004 | 0.545521623 | 0.498652776 |
| 0.275385056 | 0.674686786 | 0.487635807 |
| 0.337740682 | 0.357600274 | 0.508191639 |
| 0.337873440 | 0.483064788 | 0.502519370 |
| 0.336679836 | 0.608650318 | 0.495015454 |
| 0.367741724 | 0.734646613 | 0.476060321 |
| 0.400277030 | 0.294863662 | 0.509601662 |
| 0.400287403 | 0.420335979 | 0.505329357 |
| 0.400206464 | 0.546094584 | 0.497489805 |
| 0.399918252 | 0.668806736 | 0.492767591 |
| 0.462797604 | 0.357627636 | 0.506921482 |
| 0.462679645 | 0.483141546 | 0.499955740 |
| 0.463442691 | 0.608622571 | 0.491649323 |
| 0.431597224 | 0.734721942 | 0.475985215 |
| 0.525289533 | 0.294886876 | 0.508427966 |
| 0.525296099 | 0.420426170 | 0.502289940 |
| 0.525142548 | 0.545682775 | 0.492045511 |
| 0.524175655 | 0.674650413 | 0.486937929 |
| 0.587784221 | 0.357661482 | 0.504451402 |
| 0.587798306 | 0.483180666 | 0.495059366 |

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| 0.586351107 | 0.608773174 | 0.482570428 |
| 0.618943536 | 0.731827301 | 0.508818460 |
| 0.650270820 | 0.294910008 | 0.507081090 |
| 0.650266871 | 0.420424385 | 0.498734209 |
| 0.650045751 | 0.546199748 | 0.486620390 |
| 0.649384914 | 0.669105415 | 0.476200029 |
| 0.712754945 | 0.357681564 | 0.502430787 |
| 0.712630515 | 0.483252534 | 0.492106982 |
| 0.713299774 | 0.608796525 | 0.481097606 |
| 0.686397025 | 0.731574117 | 0.510022527 |
| 0.775231552 | 0.294910338 | 0.506396784 |
| 0.775217991 | 0.420480291 | 0.497148664 |
| 0.775157751 | 0.545894091 | 0.487445131 |
| 0.774460607 | 0.674533161 | 0.485574886 |
| 0.837690363 | 0.357681235 | 0.502011820 |
| 0.837755647 | 0.483267534 | 0.492843899 |
| 0.836716523 | 0.609080973 | 0.487817276 |
| 0.864696844 | 0.731739884 | 0.473922902 |
| 0.900192475 | 0.294902316 | 0.506651588 |
| 0.900155835 | 0.420425017 | 0.498029435 |
| 0.900142417 | 0.546318867 | 0.491161925 |
| 0.900539262 | 0.669433049 | 0.492358590 |
| 0.962662420 | 0.357661235 | 0.503216995 |
| 0.962540892 | 0.483207699 | 0.495441950 |
| 0.963731902 | 0.608843778 | 0.491521826 |
| 0.936271095 | 0.731417415 | 0.475929091 |
| 0.087680382 | 0.234060575 | 0.510899311 |
| 0.212720329 | 0.234049256 | 0.511053921 |
| 0.337773348 | 0.234051399 | 0.511047435 |
| 0.462804313 | 0.234069201 | 0.510859196 |
| 0.587798401 | 0.234093185 | 0.510586265 |
| 0.712757943 | 0.234106234 | 0.510462754 |
| 0.837709587 | 0.234101316 | 0.510529635 |
| 0.962676219 | 0.234081207 | 0.510697373 |
| 0.834623999 | 0.763547911 | 0.452776727 |
| 0.585605905 | 0.760662006 | 0.532218446 |
| 0.084687606 | 0.762006608 | 0.475193692 |
| 0.958711387 | 0.757317865 | 0.465380632 |
| 0.846413241 | 0.796590376 | 0.588890386 |
| 0.866261764 | 0.835336408 | 0.452561722 |
| 0.778193281 | 0.839968614 | 0.434689962 |
| 0.817253710 | 0.865948952 | 0.521600355 |
| 0.718020134 | 0.766655132 | 0.538299115 |
| 0.734034109 | 0.787266570 | 0.645988727 |
| 0.699502850 | 0.817588732 | 0.556988024 |
| 0.804107582 | 0.806838513 | 0.549609674 |

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Direct
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   0.092040001       0.690455032        0.493699012
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   0.150620998       0.626467004        0.491831013
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| 0.900298014 | 0.502937992 | 0.492700995 |
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| 0.962768055 | 0.314485000 | 0.499991015 |
| 0.962741979 | 0.439960998 | 0.494555011 |
| 0.963392062 | 0.565455979 | 0.491171005 |
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| 0.399453030 | 0.667522024 | 0.503750993 |
| 0.462881017 | 0.356335012 | 0.506196966 |
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| 0.650192022 | 0.545144044 | 0.499213982 |
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| 0.775270000 | 0.544627016 | 0.494654002 |

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| 0.837221001 | 0.607563956 | 0.492759998 |
| 0.865746056 | 0.730905003 | 0.500078966 |
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| 0.900250050 | 0.419043987 | 0.495184015 |
| 0.900363013 | 0.544858003 | 0.491649006 |
| 0.901142047 | 0.667864988 | 0.493514000 |
| 0.962765009 | 0.356256002 | 0.497870997 |
| 0.962712002 | 0.481776010 | 0.493022996 |
| 0.964072979 | 0.607328024 | 0.490877984 |
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| 0.087765003 | 0.232649985 | 0.504791973 |
| 0.212818993 | 0.232643996 | 0.505267032 |
| 0.337866992 | 0.232673996 | 0.505717984 |
| 0.462875022 | 0.232717017 | 0.505911000 |
| 0.587840988 | 0.232748006 | 0.505761042 |
| 0.712782020 | 0.232751989 | 0.505291993 |
| 0.837737946 | 0.232728006 | 0.504805039 |
| 0.962731035 | 0.232685012 | 0.504577981 |
| 0.835052059 | 0.762855006 | 0.504288029 |
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| 0.586730013 | 0.763786974 | 0.508125011 |
| 0.958392008 | 0.756986989 | 0.501498986 |
| 0.748178011 | 0.861550975 | 0.576467981 |
| 0.863224046 | 0.839484003 | 0.519676991 |
| 0.861066999 | 0.877102025 | 0.438962015 |
| 0.866611978 | 0.888149989 | 0.554363999 |
| 0.709927021 | 0.756896001 | 0.502839029 |
| 0.673657020 | 0.877653998 | 0.454397009 |
| 0.746379980 | 0.885788035 | 0.379704014 |
| 0.769344973 | 0.869160018 | 0.511688999 |
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| 0.727689016 | 0.877953995 | 0.445468010 |

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      0.0000000000      0.0000000000    15.0721998215
  B  N  O  H
  64  64  11  2
Direct

| | | |
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| 0.022836999 | 0.377175981 | 0.499924008 |
| 0.022866999 | 0.502460030 | 0.496359989 |
| 0.023313000 | 0.629387029 | 0.491048982 |
| 0.085363004 | 0.314420001 | 0.501689029 |
| 0.085392999 | 0.439864983 | 0.500123036 |
| 0.085009002 | 0.565224004 | 0.494841989 |
| 0.089523005 | 0.690436021 | 0.490080008 |
| 0.147905002 | 0.251536001 | 0.502439962 |
| 0.147861998 | 0.377121009 | 0.502834030 |
| 0.147892999 | 0.502685028 | 0.500262017 |
| 0.148160001 | 0.626384972 | 0.492278011 |
| 0.210407994 | 0.314427995 | 0.503959006 |
| 0.210327007 | 0.439848994 | 0.504387021 |
| 0.210932005 | 0.565189004 | 0.499766994 |
| 0.206229013 | 0.691176013 | 0.491057017 |
| 0.272924999 | 0.251551001 | 0.503302984 |
| 0.272906013 | 0.377173014 | 0.506149004 |
| 0.272886980 | 0.502417008 | 0.505457992 |
| 0.272689009 | 0.629371975 | 0.498114000 |
| 0.335426991 | 0.314462006 | 0.505700995 |
| 0.335456993 | 0.439910999 | 0.508006974 |
| 0.334791992 | 0.565374002 | 0.505414017 |
| 0.338869977 | 0.689809049 | 0.492168990 |
| 0.397930007 | 0.251583995 | 0.503670984 |
| 0.397949016 | 0.377211008 | 0.507801999 |
| 0.397876000 | 0.502884971 | 0.508395000 |
| 0.397648980 | 0.626712002 | 0.504417013 |
| 0.460440993 | 0.314500000 | 0.505850004 |
| 0.460404972 | 0.440034981 | 0.508445967 |
| 0.460799010 | 0.565597022 | 0.506447024 |
| 0.456095970 | 0.691923039 | 0.492462991 |
| 0.522913983 | 0.251614983 | 0.503364011 |
| 0.522950004 | 0.377297023 | 0.506690976 |
| 0.522914982 | 0.502747994 | 0.506703029 |
| 0.522393993 | 0.630039990 | 0.500621032 |
| 0.585413002 | 0.314527005 | 0.504324981 |
| 0.585466961 | 0.440108002 | 0.505473969 |
| 0.584783950 | 0.565850975 | 0.502311990 |
| 0.588098985 | 0.691089970 | 0.494434000 |
| 0.647882995 | 0.251626027 | 0.502560973 |
| 0.647903027 | 0.377297023 | 0.503591006 |
| 0.647819994 | 0.503112001 | 0.502097018 |
| 0.647674960 | 0.627320017 | 0.496044000 |
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| 0.707622990 | 0.691377989 | 0.493333986 |
| 0.772865995 | 0.251603995 | 0.501738003 |
| 0.772842013 | 0.377311996 | 0.500450003 |
| 0.772827976 | 0.502767005 | 0.497658018 |
| 0.772919003 | 0.629645983 | 0.493402005 |
| 0.835346980 | 0.314497006 | 0.500466992 |
| 0.835350977 | 0.440052975 | 0.498046993 |
| 0.834994007 | 0.565614000 | 0.493912023 |
| 0.838835027 | 0.690254979 | 0.492157980 |
| 0.897862986 | 0.251569984 | 0.501362979 |
| 0.897813023 | 0.377220019 | 0.498986007 |
| 0.897862034 | 0.502896014 | 0.495360992 |
| 0.898307033 | 0.626963043 | 0.491261012 |
| 0.960349966 | 0.314455990 | 0.500294033 |
| 0.960278020 | 0.439929982 | 0.497603001 |
| 0.960959984 | 0.565433013 | 0.492850005 |
| 0.958131061 | 0.691402989 | 0.491239024 |
| 0.022856001 | 0.293434007 | 0.501031995 |
| 0.022825999 | 0.418976982 | 0.499025996 |
| 0.022937000 | 0.544197021 | 0.494394991 |
| 0.024063000 | 0.672814003 | 0.490561015 |
| 0.085340003 | 0.356189986 | 0.501378007 |
| 0.085444002 | 0.481667001 | 0.498818996 |
| 0.084739002 | 0.607040005 | 0.492295000 |
| 0.114787003 | 0.732394988 | 0.492226980 |
| 0.147892000 | 0.293433018 | 0.502696980 |
| 0.147857990 | 0.418905994 | 0.502524021 |
| 0.147963006 | 0.544568006 | 0.498169016 |
| 0.148448998 | 0.667059996 | 0.489250995 |
| 0.210401998 | 0.356198008 | 0.504489018 |
| 0.210305999 | 0.481652001 | 0.503653995 |
| 0.211474003 | 0.607029950 | 0.496594987 |
| 0.178320007 | 0.733053003 | 0.493192000 |
| 0.272924999 | 0.293444007 | 0.504535018 |
| 0.272899994 | 0.418972998 | 0.506613022 |
| 0.272884006 | 0.544168999 | 0.504059959 |
| 0.272496011 | 0.673239988 | 0.493431997 |
| 0.335433986 | 0.356238997 | 0.506946032 |
| 0.335481998 | 0.481727989 | 0.508004000 |
| 0.334161013 | 0.607294013 | 0.503578003 |
| 0.369320015 | 0.731494997 | 0.477200007 |
| 0.397941998 | 0.293478017 | 0.505345998 |
| 0.397955012 | 0.419005004 | 0.508727029 |
| 0.397810002 | 0.544816026 | 0.507744009 |
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| 0.460464023 | 0.356278996 | 0.507210010 |
| 0.460350013 | 0.481875020 | 0.508580044 |
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| 0.434823992 | 0.732044991 | 0.477854985 |
| 0.522928020 | 0.293507000 | 0.504719018 |
| 0.522957998 | 0.419122997 | 0.507351996 |
| 0.522872966 | 0.544532017 | 0.505745002 |
| 0.521772983 | 0.673443997 | 0.496055009 |
| 0.585421995 | 0.356312979 | 0.505087018 |
| 0.585473004 | 0.481946998 | 0.505105969 |
| 0.584148999 | 0.607787030 | 0.499878989 |
| 0.613461986 | 0.731630984 | 0.495748986 |
| 0.647895985 | 0.293520984 | 0.503014993 |
| 0.647893035 | 0.419113986 | 0.503563988 |
| 0.647739007 | 0.545050968 | 0.500693986 |
| 0.647499996 | 0.668122018 | 0.493420007 |
| 0.710380015 | 0.356313996 | 0.501977968 |
| 0.710241975 | 0.481974030 | 0.500280967 |
| 0.711089006 | 0.607581043 | 0.495485989 |
| 0.684759017 | 0.730435008 | 0.494343993 |
| 0.772862950 | 0.293498017 | 0.501286988 |
| 0.772811988 | 0.419138024 | 0.499733016 |
| 0.772840967 | 0.544543006 | 0.496162005 |
| 0.773150972 | 0.672763015 | 0.492832984 |
| 0.835312054 | 0.356281991 | 0.499748993 |
| 0.835386950 | 0.481881009 | 0.496748015 |
| 0.834744956 | 0.607485989 | 0.492492002 |
| 0.862677979 | 0.730730994 | 0.493124012 |
| 0.897845951 | 0.293466973 | 0.500490023 |
| 0.897789041 | 0.419012998 | 0.497916997 |
| 0.897930935 | 0.544806026 | 0.493645989 |
| 0.898650965 | 0.667775978 | 0.490891019 |
| 0.960321035 | 0.356233008 | 0.499494000 |
| 0.960258035 | 0.481736011 | 0.496132994 |
| 0.961632051 | 0.607289013 | 0.491230989 |
| 0.934053047 | 0.730437975 | 0.492608015 |
| 0.085392000 | 0.232614985 | 0.502075030 |
| 0.210424005 | 0.232620013 | 0.502556986 |
| 0.335441005 | 0.232643996 | 0.502883004 |
| 0.460434997 | 0.232675012 | 0.502891008 |
| 0.585401011 | 0.232693996 | 0.502574039 |
| 0.710367024 | 0.232690012 | 0.502126978 |
| 0.835350977 | 0.232658996 | 0.501779004 |
| 0.960362052 | 0.232628996 | 0.501766033 |
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   0.031032738        0.631052012        0.508078948
   0.093411156        0.315821800        0.501247473
   0.093377194        0.441308072        0.506059124
   0.092888578        0.566881295        0.510333897
   0.097756863        0.693018082        0.503579490
   0.155960345        0.252923157        0.499305508
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   0.155829432        0.504168694        0.508691501
   0.155963807        0.628324348        0.512769272
   0.218444863        0.315809630        0.501887076
   0.218330401        0.441273567        0.506091109
   0.218738048        0.566701186        0.508094419
   0.214791630        0.692222431        0.497698829
   0.280986064        0.252925547        0.499258116
   0.280920304        0.378564345        0.503352812
   0.280859659        0.503853807        0.505359760
   0.280592360        0.630508831        0.501753378
   0.343467763        0.315831882        0.500747801
   0.343452988        0.441308429        0.502905372
   0.342837688        0.566669154        0.501018992
   0.346373200        0.691076344        0.498576626
   0.406002207        0.252947992        0.498662615
   0.405946868        0.378574977        0.500572089
   0.405907706        0.504197045        0.500493409
   0.405756154        0.627923198        0.493367173
   0.468478671        0.315859327        0.498757019
   0.468390214        0.441345187        0.499157131
   0.468846633        0.566848218        0.497757231
   0.463507404        0.692790667        0.502144979
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| 0.530998959 | 0.252972497 | 0.497786147 |
| 0.530968601 | 0.378641955 | 0.497701392 |
| 0.530894799 | 0.503996827 | 0.497835089 |
| 0.530484060 | 0.631382943 | 0.498901948 |
| 0.593466573 | 0.315892843 | 0.496863331 |
| 0.593485273 | 0.441419555 | 0.496709639 |
| 0.592728556 | 0.567055359 | 0.498192048 |
| 0.596093172 | 0.693554011 | 0.505321859 |
| 0.655976012 | 0.252986590 | 0.496979945 |
| 0.655965734 | 0.378650718 | 0.495948646 |
| 0.655867760 | 0.504418801 | 0.497158820 |
| 0.655539102 | 0.628300227 | 0.501711618 |
| 0.718462041 | 0.315898145 | 0.496043019 |
| 0.718377295 | 0.441470104 | 0.496437309 |
| 0.718794696 | 0.567065084 | 0.499619535 |
| 0.714004388 | 0.691732931 | 0.505820392 |
| 0.780945404 | 0.252972497 | 0.496839952 |
| 0.780945166 | 0.378691844 | 0.496379129 |
| 0.780872412 | 0.504102980 | 0.498905902 |
| 0.780762066 | 0.631336405 | 0.502941121 |
| 0.843421297 | 0.315888887 | 0.496977730 |
| 0.843452131 | 0.441446752 | 0.498835447 |
| 0.842783300 | 0.567017996 | 0.502297406 |
| 0.847069034 | 0.693836975 | 0.505151083 |
| 0.905936732 | 0.252954723 | 0.497526377 |
| 0.905902758 | 0.378623960 | 0.499079810 |
| 0.905865072 | 0.504363637 | 0.502688532 |
| 0.905766765 | 0.628218195 | 0.503913986 |
| 0.968408010 | 0.315850453 | 0.499174373 |
| 0.968321884 | 0.441389583 | 0.502815491 |
| 0.968843968 | 0.566938712 | 0.506324874 |
| 0.964746474 | 0.691453153 | 0.504676150 |
| 0.030910359 | 0.294842316 | 0.499700114 |
| 0.030831859 | 0.420418121 | 0.504028069 |
| 0.030815184 | 0.545790851 | 0.508213753 |
| 0.031108645 | 0.674910136 | 0.505044277 |
| 0.093361200 | 0.357604010 | 0.502899455 |
| 0.093371710 | 0.483141326 | 0.507813167 |
| 0.092433944 | 0.608834492 | 0.511810010 |
| 0.123785983 | 0.733405472 | 0.479715518 |
| 0.155930368 | 0.294824707 | 0.501040030 |
| 0.155842041 | 0.420329083 | 0.505917264 |
| 0.155751134 | 0.546084639 | 0.510167013 |
| 0.156075937 | 0.669142227 | 0.512361409 |
| 0.218412435 | 0.357592966 | 0.503521278 |
| 0.218262072 | 0.483092920 | 0.507345669 |

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| 0.219087381 | 0.608527078 | 0.508383991 |
| 0.186466592 | 0.731629226 | 0.469959910 |
| 0.280964128 | 0.294824844 | 0.500852835 |
| 0.280905744 | 0.420376281 | 0.504471301 |
| 0.280793685 | 0.545596018 | 0.505127134 |
| 0.280421940 | 0.673837070 | 0.498230107 |
| 0.343440402 | 0.357616180 | 0.501721615 |
| 0.343474543 | 0.483121821 | 0.503010627 |
| 0.342293882 | 0.608466694 | 0.498010516 |
| 0.372254574 | 0.731526535 | 0.514708801 |
| 0.405986362 | 0.294852454 | 0.499487862 |
| 0.405932830 | 0.420372627 | 0.500884883 |
| 0.405894336 | 0.546093430 | 0.499358056 |
| 0.405725415 | 0.668627617 | 0.490366543 |
| 0.468479670 | 0.357650740 | 0.498976706 |
| 0.468357143 | 0.483163414 | 0.498966930 |
| 0.469289205 | 0.608717296 | 0.496118252 |
| 0.436736365 | 0.733877555 | 0.517890995 |
| 0.530986540 | 0.294877206 | 0.497751220 |
| 0.530963462 | 0.420460263 | 0.497650678 |
| 0.530874719 | 0.545763488 | 0.497877166 |
| 0.529997045 | 0.674999585 | 0.502585839 |
| 0.593473092 | 0.357684696 | 0.496594165 |
| 0.593513300 | 0.483261545 | 0.496888293 |
| 0.592128149 | 0.608945260 | 0.499422311 |
| 0.616630035 | 0.734136179 | 0.507473007 |
| 0.655965211 | 0.294896492 | 0.496389443 |
| 0.655956693 | 0.420469439 | 0.495966901 |
| 0.655832168 | 0.546390185 | 0.498036078 |
| 0.655502606 | 0.669043767 | 0.504575608 |
| 0.718476411 | 0.357701042 | 0.495691470 |
| 0.718318101 | 0.483328687 | 0.497081246 |
| 0.719256206 | 0.609029270 | 0.501292935 |
| 0.682267507 | 0.734117552 | 0.507972364 |
| 0.780942549 | 0.294885063 | 0.496345847 |
| 0.780925800 | 0.420533175 | 0.496778576 |
| 0.780807270 | 0.545904146 | 0.500080421 |
| 0.780610941 | 0.675167550 | 0.504787132 |
| 0.843412732 | 0.357690136 | 0.497140122 |
| 0.843460792 | 0.483305281 | 0.499955297 |
| 0.842271494 | 0.608933557 | 0.503022966 |
| 0.868415576 | 0.734341341 | 0.508103309 |
| 0.905910561 | 0.294871629 | 0.497729232 |
| 0.905884295 | 0.420446939 | 0.500087444 |
| 0.905817393 | 0.546333922 | 0.503803384 |
| 0.905919222 | 0.668992339 | 0.503304123 |

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| 0.968383933 | 0.357644971 | 0.500204564 |
| 0.968258789 | 0.483247094 | 0.504240922 |
| 0.969349779 | 0.608899107 | 0.506258658 |
| 0.933997089 | 0.733801896 | 0.508381555 |
| 0.093447534 | 0.234021427 | 0.498415657 |
| 0.218476316 | 0.234014669 | 0.498601208 |
| 0.343503426 | 0.234032581 | 0.498440935 |
| 0.468509124 | 0.234049696 | 0.498080022 |
| 0.593494695 | 0.234060960 | 0.497492810 |
| 0.718457092 | 0.234064916 | 0.497053216 |
| 0.843435097 | 0.234054778 | 0.497156953 |
| 0.968429137 | 0.234024531 | 0.497777415 |
| 0.969372619 | 0.763258299 | 0.512469892 |
| 0.264520144 | 0.755132283 | 0.559740684 |
| 0.716757321 | 0.763913292 | 0.509867602 |
| 0.245055570 | 0.780729878 | 0.566240605 |
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IM26
E+ZPE = -1191.50695 eV
1.0

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| 0.0000000000 | 0.0000000000 | 15.0721998215 |

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Direct

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| 0.032871000 | 0.377518010 | 0.503943029 |
| 0.032851000 | 0.502860026 | 0.499850010 |
| 0.032995998 | 0.629962958 | 0.496965993 |
| 0.095366997 | 0.314752992 | 0.505110967 |
| 0.095409001 | 0.440263001 | 0.501513001 |
| 0.094888999 | 0.565754987 | 0.498105996 |
| 0.099326000 | 0.691401011 | 0.496885983 |
| 0.157884995 | 0.251848992 | 0.505572011 |
| 0.157874004 | 0.377491005 | 0.503017018 |
| 0.157864999 | 0.503170023 | 0.499009007 |
| 0.157919006 | 0.627026999 | 0.497693989 |
| 0.220394994 | 0.314754998 | 0.504066002 |
| 0.220326997 | 0.440266984 | 0.500211999 |
| 0.220882009 | 0.565780976 | 0.497208015 |
| 0.216625015 | 0.691373978 | 0.496936001 |
| 0.282912998 | 0.251853992 | 0.504786025 |
| 0.282880998 | 0.377530015 | 0.501564032 |

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| 0.282855993 | 0.502879971 | 0.497655993 |
| 0.282831012 | 0.630089989 | 0.496073992 |
| 0.345393007 | 0.314765986 | 0.502713969 |
| 0.345420986 | 0.440295995 | 0.498953010 |
| 0.344832975 | 0.565838997 | 0.495685997 |
| 0.348623010 | 0.692421001 | 0.495963009 |
| 0.407922003 | 0.251866025 | 0.503951002 |
| 0.407874991 | 0.377523010 | 0.500436019 |
| 0.407868996 | 0.503245022 | 0.496776994 |
| 0.407748990 | 0.627129964 | 0.493974000 |
| 0.470393995 | 0.314779997 | 0.501869992 |
| 0.470322001 | 0.440311022 | 0.498583997 |
| 0.470858979 | 0.565890041 | 0.495266998 |
| 0.466319007 | 0.690587008 | 0.494733000 |
| 0.532911000 | 0.251873992 | 0.503535989 |
| 0.532871030 | 0.377558999 | 0.500338008 |
| 0.532855993 | 0.502942992 | 0.497233989 |
| 0.532888017 | 0.630189988 | 0.494627997 |
| 0.595379993 | 0.314783019 | 0.502042001 |
| 0.595407021 | 0.440320995 | 0.499383018 |
| 0.594837020 | 0.565886964 | 0.496311996 |
| 0.599137029 | 0.692732975 | 0.493063016 |
| 0.657890955 | 0.251879019 | 0.503790033 |
| 0.657856981 | 0.377532982 | 0.501350989 |
| 0.657866022 | 0.503247000 | 0.498423978 |
| 0.657814013 | 0.627125954 | 0.495938997 |
| 0.720370988 | 0.314779008 | 0.503121008 |
| 0.720309035 | 0.440302011 | 0.500696011 |
| 0.720886982 | 0.565834987 | 0.497169987 |
| 0.716668007 | 0.690415032 | 0.493306019 |
| 0.782866010 | 0.251879019 | 0.504589971 |
| 0.782850973 | 0.377539988 | 0.502784013 |
| 0.782863012 | 0.502898981 | 0.499377007 |
| 0.783027983 | 0.629945980 | 0.495480009 |
| 0.845354988 | 0.314772992 | 0.504458014 |
| 0.845400002 | 0.440284017 | 0.501739015 |
| 0.844915985 | 0.565791031 | 0.497496005 |
| 0.849621974 | 0.691779963 | 0.494465004 |
| 0.907855958 | 0.251868992 | 0.505456980 |
| 0.907861002 | 0.377503999 | 0.503834008 |
| 0.907873944 | 0.503184967 | 0.499873990 |
| 0.907977010 | 0.627099965 | 0.495424012 |
| 0.970365968 | 0.314757992 | 0.505271967 |
| 0.970314959 | 0.440263990 | 0.502094993 |
| 0.970910036 | 0.565792020 | 0.497961985 |
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| 0.032866001 | 0.544646961 | 0.498661001 |
| 0.033119998 | 0.673740038 | 0.496551012 |
| 0.095365004 | 0.356555999 | 0.504269015 |
| 0.095430003 | 0.482106007 | 0.500150022 |
| 0.094420000 | 0.607653021 | 0.497637011 |
| 0.126425001 | 0.733489976 | 0.495485008 |
| 0.157882010 | 0.293772025 | 0.505122009 |
| 0.157869995 | 0.419312006 | 0.501636986 |
| 0.157879000 | 0.545111022 | 0.498099004 |
| 0.157861989 | 0.667763011 | 0.497952019 |
| 0.220391996 | 0.356559982 | 0.502998004 |
| 0.220283007 | 0.482107985 | 0.498879992 |
| 0.221387986 | 0.607674998 | 0.497029014 |
| 0.189928991 | 0.733502998 | 0.495588018 |
| 0.282902982 | 0.293772025 | 0.503907975 |
| 0.282887993 | 0.419367994 | 0.500188999 |
| 0.282873004 | 0.544657016 | 0.496697997 |
| 0.282599995 | 0.673668994 | 0.496338001 |
| 0.345380992 | 0.356572015 | 0.501506990 |
| 0.345465976 | 0.482145018 | 0.497609993 |
| 0.344359997 | 0.607717965 | 0.495004001 |
| 0.368970992 | 0.733003003 | 0.498582004 |
| 0.407905016 | 0.293785981 | 0.502746997 |
| 0.407880987 | 0.419346978 | 0.499202023 |
| 0.407891978 | 0.545206022 | 0.495611018 |
| 0.407819985 | 0.667893998 | 0.493617009 |
| 0.470388998 | 0.356588004 | 0.500720023 |
| 0.470290977 | 0.482169962 | 0.497370976 |
| 0.471397003 | 0.607860986 | 0.494302011 |
| 0.434635990 | 0.732994047 | 0.498192997 |
| 0.532895012 | 0.293791009 | 0.502303006 |
| 0.532872029 | 0.419405027 | 0.499341985 |
| 0.532856993 | 0.544750971 | 0.496132994 |
| 0.532784999 | 0.674005969 | 0.494156987 |
| 0.595359961 | 0.356591988 | 0.501125988 |
| 0.595452034 | 0.482182984 | 0.498352004 |
| 0.594364994 | 0.607808019 | 0.495618990 |
| 0.620325974 | 0.733210968 | 0.489010998 |
| 0.657877965 | 0.293797986 | 0.502868008 |
| 0.657855981 | 0.419362005 | 0.500520996 |
| 0.657871018 | 0.545222999 | 0.497334974 |
| 0.657971990 | 0.667893998 | 0.495202997 |
| 0.720354952 | 0.356588004 | 0.502453977 |
| 0.720269017 | 0.482163039 | 0.499599003 |

| | | |
|---|---|---|
| 0.721403023 | 0.607801975 | 0.496210979 |
| 0.685937988 | 0.732720973 | 0.488941017 |
| 0.782863012 | 0.293794003 | 0.504086028 |
| 0.782845977 | 0.419385000 | 0.501882014 |
| 0.782870007 | 0.544710972 | 0.498017982 |
| 0.783070047 | 0.673856959 | 0.494246994 |
| 0.845341950 | 0.356577015 | 0.503883014 |
| 0.845433025 | 0.482136996 | 0.500417006 |
| 0.844458994 | 0.607712965 | 0.495989996 |
| 0.877023968 | 0.733362011 | 0.496476001 |
| 0.907851961 | 0.293789003 | 0.505254978 |
| 0.907849011 | 0.419327995 | 0.502743011 |
| 0.907884984 | 0.545140967 | 0.498414993 |
| 0.907981958 | 0.667823010 | 0.494146990 |
| 0.970368062 | 0.356563993 | 0.504623000 |
| 0.970266995 | 0.482109029 | 0.500683008 |
| 0.971424031 | 0.607699998 | 0.496726976 |
| 0.940218988 | 0.733156958 | 0.497082005 |
| 0.095372998 | 0.232954982 | 0.505934000 |
| 0.220403012 | 0.232958004 | 0.505505985 |
| 0.345425007 | 0.232968993 | 0.504809974 |
| 0.470424020 | 0.232971987 | 0.504216024 |
| 0.595403024 | 0.232980998 | 0.504051037 |
| 0.720377983 | 0.232983004 | 0.504442986 |
| 0.845352038 | 0.232975009 | 0.505199013 |
| 0.970351027 | 0.232963004 | 0.505815995 |
| 0.469137985 | 0.762740007 | 0.500916014 |
| 0.721299005 | 0.762174024 | 0.485051992 |
| 0.080385997 | 0.813360973 | 0.467384005 |
| 0.123088007 | 0.826611003 | 0.469862026 |
| 0.091646000 | 0.786297953 | 0.480356006 |

IM27 (10O)
E+ZPE = -1177.72839 eV
1.0

| | | |
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| 20.0422000885 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 34.7140998840 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 15.0721998215 |

  B   N   O
 64   64   10
Direct

| | | |
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| 0.022934999 | 0.250232992 | 0.501966010 |
| 0.022908000 | 0.375912010 | 0.498894988 |
| 0.022910001 | 0.501285042 | 0.497516981 |
| 0.023027999 | 0.628541983 | 0.496094998 |

| | | |
|---|---|---|
| 0.085417005 | 0.313138998 | 0.500736000 |
| 0.085449004 | 0.438662000 | 0.499190982 |
| 0.084912003 | 0.564203959 | 0.498044019 |
| 0.089355999 | 0.689880037 | 0.495224004 |
| 0.147927996 | 0.250230987 | 0.502406015 |
| 0.147908000 | 0.375876983 | 0.500649979 |
| 0.147899006 | 0.501577017 | 0.499807015 |
| 0.147939999 | 0.625443993 | 0.498005992 |
| 0.210430001 | 0.313136003 | 0.501878977 |
| 0.210355010 | 0.438652001 | 0.501107986 |
| 0.210923012 | 0.564150993 | 0.500092032 |
| 0.206631996 | 0.689850972 | 0.496890001 |
| 0.272929019 | 0.250225987 | 0.502743011 |
| 0.272920002 | 0.375894016 | 0.502008023 |
| 0.272911985 | 0.501243998 | 0.501192995 |
| 0.272882007 | 0.628335007 | 0.499712990 |
| 0.335424993 | 0.313125014 | 0.502689007 |
| 0.335467984 | 0.438638979 | 0.501743982 |
| 0.334905002 | 0.564158026 | 0.500846982 |
| 0.338961980 | 0.689828005 | 0.498636989 |
| 0.397933980 | 0.250222003 | 0.502857030 |
| 0.397926010 | 0.375865994 | 0.502331004 |
| 0.397922013 | 0.501551962 | 0.500798989 |
| 0.397880996 | 0.625464047 | 0.500756026 |
| 0.460435996 | 0.313127981 | 0.502732982 |
| 0.460385986 | 0.438643979 | 0.500921012 |
| 0.460900981 | 0.564143026 | 0.499356000 |
| 0.456195990 | 0.690128002 | 0.499062979 |
| 0.522943009 | 0.250216014 | 0.502628043 |
| 0.522935967 | 0.375901021 | 0.501470039 |
| 0.522928020 | 0.501258009 | 0.498751008 |
| 0.522804970 | 0.628290997 | 0.497842999 |
| 0.585435985 | 0.313123998 | 0.501913018 |
| 0.585473004 | 0.438654006 | 0.499092022 |
| 0.584909999 | 0.564189948 | 0.496191997 |
| 0.589192973 | 0.688745983 | 0.498736993 |
| 0.647946994 | 0.250222003 | 0.502133021 |
| 0.647924011 | 0.375875005 | 0.499885000 |
| 0.647908975 | 0.501598006 | 0.496343000 |
| 0.647986012 | 0.625476025 | 0.493666996 |
| 0.710439018 | 0.313134025 | 0.500599012 |
| 0.710368975 | 0.438672000 | 0.497259994 |
| 0.710941974 | 0.564230003 | 0.494310996 |
| 0.706731992 | 0.691025026 | 0.497437003 |
| 0.772940987 | 0.250225987 | 0.501716964 |
| 0.772916957 | 0.375910993 | 0.498337008 |

| | | |
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| 0.772918004 | 0.501297020 | 0.495301989 |
| 0.772921049 | 0.628524016 | 0.494258985 |
| 0.835425017 | 0.313134987 | 0.499608019 |
| 0.835449950 | 0.438672000 | 0.496523994 |
| 0.834915019 | 0.564252036 | 0.494680989 |
| 0.839538975 | 0.688937025 | 0.494363987 |
| 0.897939976 | 0.250232992 | 0.501656000 |
| 0.897909998 | 0.375887010 | 0.497854008 |
| 0.897896960 | 0.501619983 | 0.495822985 |
| 0.898079966 | 0.625491959 | 0.495409016 |
| 0.960429049 | 0.313138998 | 0.499707992 |
| 0.960357008 | 0.438672989 | 0.497233989 |
| 0.960963029 | 0.564243025 | 0.496042007 |
| 0.957277035 | 0.690779973 | 0.494010002 |
| 0.022924001 | 0.292142976 | 0.500679022 |
| 0.022901000 | 0.417742022 | 0.498317994 |
| 0.022912000 | 0.543050989 | 0.497128005 |
| 0.023221999 | 0.672085000 | 0.494974990 |
| 0.085399000 | 0.354936015 | 0.499994021 |
| 0.085484995 | 0.480494980 | 0.498851012 |
| 0.084434998 | 0.606073037 | 0.497420014 |
| 0.116595002 | 0.731694006 | 0.494161986 |
| 0.147924999 | 0.292145998 | 0.501641985 |
| 0.147899006 | 0.417689001 | 0.500415993 |
| 0.147916005 | 0.543501039 | 0.499457016 |
| 0.148047002 | 0.666120995 | 0.496881997 |
| 0.210421983 | 0.354930988 | 0.501555964 |
| 0.210324009 | 0.480487013 | 0.500927973 |
| 0.211446000 | 0.606019026 | 0.499491975 |
| 0.179943990 | 0.731594007 | 0.495078000 |
| 0.272927996 | 0.292138992 | 0.502472991 |
| 0.272915982 | 0.417726995 | 0.501806971 |
| 0.272942010 | 0.543012967 | 0.500957015 |
| 0.272902991 | 0.672028022 | 0.498430021 |
| 0.335420996 | 0.354923021 | 0.502551988 |
| 0.335514997 | 0.480478991 | 0.501426981 |
| 0.334461978 | 0.606050015 | 0.500727996 |
| 0.365531004 | 0.731505986 | 0.495393989 |
| 0.397933005 | 0.292138003 | 0.502923025 |
| 0.397938025 | 0.417683012 | 0.501833989 |
| 0.397939000 | 0.543497962 | 0.500573988 |
| 0.397915994 | 0.666194950 | 0.500949011 |
| 0.460445989 | 0.354930027 | 0.502405003 |
| 0.460365002 | 0.480493002 | 0.500257018 |
| 0.461403032 | 0.606066004 | 0.499509977 |
| 0.428834014 | 0.731769994 | 0.495446000 |

| | | |
|---|---|---|
| 0.522938013 | 0.292133003 | 0.502637977 |
| 0.522938013 | 0.417737984 | 0.500583004 |
| 0.522941010 | 0.543061977 | 0.498032978 |
| 0.522777990 | 0.672209009 | 0.498797008 |
| 0.585425040 | 0.354929010 | 0.501246999 |
| 0.585509025 | 0.480511023 | 0.497974988 |
| 0.584411992 | 0.606156992 | 0.495507976 |
| 0.620019014 | 0.730947035 | 0.506203009 |
| 0.647942997 | 0.292138992 | 0.501652014 |
| 0.647923012 | 0.417699989 | 0.498708994 |
| 0.647907024 | 0.543568016 | 0.495240012 |
| 0.647836981 | 0.666257971 | 0.493916990 |
| 0.710429025 | 0.354934999 | 0.499599003 |
| 0.710322962 | 0.480528990 | 0.496032009 |
| 0.711413048 | 0.606149025 | 0.493580026 |
| 0.685585967 | 0.731430986 | 0.505129981 |
| 0.772931993 | 0.292138992 | 0.500535011 |
| 0.772903967 | 0.417751005 | 0.497182009 |
| 0.772916957 | 0.543097966 | 0.494486011 |
| 0.773032014 | 0.672331975 | 0.495128998 |
| 0.835407030 | 0.354936015 | 0.498367981 |
| 0.835474027 | 0.480524979 | 0.495687009 |
| 0.834401024 | 0.606212980 | 0.494621986 |
| 0.871141053 | 0.731314999 | 0.490888013 |
| 0.897930935 | 0.292145009 | 0.500114019 |
| 0.897896960 | 0.417704989 | 0.496955015 |
| 0.897884018 | 0.543579994 | 0.495360992 |
| 0.897997932 | 0.666248960 | 0.495357005 |
| 0.960418010 | 0.354936977 | 0.498546982 |
| 0.960303049 | 0.480517012 | 0.496689993 |
| 0.961467032 | 0.606105015 | 0.495781983 |
| 0.936767960 | 0.731363020 | 0.491237000 |
| 0.085430001 | 0.231322993 | 0.502676004 |
| 0.210430001 | 0.231321015 | 0.502852981 |
| 0.335433986 | 0.231317993 | 0.502874019 |
| 0.460440993 | 0.231318982 | 0.502735988 |
| 0.585448023 | 0.231317993 | 0.502449990 |
| 0.710443967 | 0.231317993 | 0.502241029 |
| 0.835439958 | 0.231322993 | 0.502282979 |
| 0.960439042 | 0.231327993 | 0.502457014 |
| 0.836551028 | 0.761039970 | 0.487298020 |
| 0.584730990 | 0.760306021 | 0.513835023 |

IM28
E+ZPE = -1187.48110 eV

1.0
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     0.0000000000       34.7140998840        0.0000000000
     0.0000000000        0.0000000000       15.0721998215
   B   N   O
  64   64   12
Direct
   0.032526000         0.251723004         0.486676988
   0.032545001         0.377368973         0.494866001
   0.032561001         0.502702005         0.503522986
   0.032673999         0.629900980         0.513153976
   0.095037994         0.314599010         0.491358011
   0.095092994         0.440080997         0.500217978
   0.094548998         0.565574000         0.509334014
   0.099004997         0.691204035         0.518320023
   0.157541004         0.251710010         0.487128003
   0.157543002         0.377308012         0.496435000
   0.157541004         0.502953981         0.505609976
   0.157590003         0.626770023         0.514448999
   0.220052013         0.314582994         0.492060001
   0.219997007         0.440048003         0.501297997
   0.220559989         0.565482957         0.510902001
   0.216277015         0.691136014         0.519444998
   0.282562999         0.251706988         0.487257999
   0.282546987         0.377321996         0.496581004
   0.282552983         0.502612006         0.505917011
   0.282521982         0.629614994         0.516179030
   0.345066015         0.314592005         0.491708009
   0.345090996         0.440048003         0.500455033
   0.344556992         0.565482957         0.510839992
   0.348592010         0.691062992         0.520191027
   0.407575026         0.251718004         0.486995002
   0.407564034         0.377321996         0.495245011
   0.407545001         0.502945025         0.504189006
   0.407532010         0.626742001         0.516552977
   0.470078993         0.314617004         0.490527986
   0.470005001         0.440095997         0.498088975
   0.470537030         0.565517023         0.508201003
   0.465812007         0.691407000         0.519743018
   0.532574015         0.251730999         0.486505991
   0.532567020         0.377394000         0.493160996
   0.532545988         0.502712005         0.500915001
   0.532423033         0.629639994         0.512462014
   0.595067038         0.314644010         0.489237012
   0.595102011         0.440158002         0.495514019
   0.594546952         0.565633011         0.504208969
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| | | |
|---|---|---|
| 0.598806991 | 0.690023992 | 0.518786002 |
| 0.657561013 | 0.251744982 | 0.486099014 |
| 0.657562963 | 0.377402984 | 0.491586998 |
| 0.657561013 | 0.503092990 | 0.498465011 |
| 0.657625012 | 0.626911011 | 0.507542007 |
| 0.720055987 | 0.314657993 | 0.488580990 |
| 0.720027008 | 0.440193001 | 0.494473008 |
| 0.720597960 | 0.565702955 | 0.502677966 |
| 0.716344012 | 0.692326002 | 0.518276997 |
| 0.782544013 | 0.251747015 | 0.485965981 |
| 0.782558955 | 0.377436994 | 0.491473991 |
| 0.782589027 | 0.502797004 | 0.498628004 |
| 0.782569994 | 0.629935046 | 0.509374035 |
| 0.845039035 | 0.314654999 | 0.488913999 |
| 0.845128016 | 0.440178990 | 0.495514019 |
| 0.844579951 | 0.565701032 | 0.504378985 |
| 0.849165936 | 0.690288000 | 0.516198993 |
| 0.907528965 | 0.251740010 | 0.486198006 |
| 0.907551995 | 0.377382984 | 0.492817008 |
| 0.907579974 | 0.503082990 | 0.500822021 |
| 0.907717014 | 0.626871011 | 0.511452007 |
| 0.970038975 | 0.314630988 | 0.490052990 |
| 0.970016992 | 0.440136985 | 0.497844992 |
| 0.970617018 | 0.565652021 | 0.506968020 |
| 0.966908945 | 0.692117982 | 0.516967009 |
| 0.032530999 | 0.293624005 | 0.489373999 |
| 0.032542999 | 0.419187996 | 0.497700981 |
| 0.032558003 | 0.544450974 | 0.506599007 |
| 0.032868002 | 0.673426964 | 0.516350976 |
| 0.095032998 | 0.356383006 | 0.494340987 |
| 0.095123002 | 0.481900020 | 0.503257996 |
| 0.094083003 | 0.607424012 | 0.512385010 |
| 0.126270998 | 0.732999981 | 0.522037038 |
| 0.157545001 | 0.293603977 | 0.490295993 |
| 0.157542003 | 0.419100992 | 0.499535001 |
| 0.157548998 | 0.544859981 | 0.508797991 |
| 0.157693996 | 0.667439992 | 0.517010984 |
| 0.220051014 | 0.356361990 | 0.495242005 |
| 0.219968005 | 0.481866010 | 0.504495029 |
| 0.221086998 | 0.607328024 | 0.514064010 |
| 0.189614002 | 0.732864049 | 0.522648990 |
| 0.282564998 | 0.293599994 | 0.490489990 |
| 0.282550009 | 0.419133986 | 0.499636999 |
| 0.282585006 | 0.544355975 | 0.509414024 |
| 0.282533997 | 0.673289987 | 0.518873984 |
| 0.345055998 | 0.356371990 | 0.494677983 |

| | | |
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| 0.345142981 | 0.481864031 | 0.503651970 |
| 0.344110994 | 0.607340991 | 0.514926020 |
| 0.375077002 | 0.732774984 | 0.519021982 |
| 0.407579974 | 0.293619994 | 0.489827008 |
| 0.407561988 | 0.419125991 | 0.497994982 |
| 0.407581021 | 0.544858992 | 0.507944998 |
| 0.407562987 | 0.667433014 | 0.520772987 |
| 0.470083989 | 0.356406989 | 0.492998983 |
| 0.469984017 | 0.481927987 | 0.500976978 |
| 0.471032991 | 0.607397034 | 0.512640003 |
| 0.438367997 | 0.733073992 | 0.518630982 |
| 0.532576965 | 0.293639994 | 0.488728987 |
| 0.532563975 | 0.419223985 | 0.495419994 |
| 0.532571017 | 0.544489985 | 0.504208019 |
| 0.532386013 | 0.673511963 | 0.517417012 |
| 0.595062993 | 0.356446000 | 0.491166006 |
| 0.595138032 | 0.482007986 | 0.497910005 |
| 0.594039999 | 0.607577032 | 0.507599998 |
| 0.629588019 | 0.732020980 | 0.530886977 |
| 0.657561013 | 0.293659004 | 0.487860998 |
| 0.657566009 | 0.419223023 | 0.493532982 |
| 0.657556016 | 0.545052012 | 0.501217007 |
| 0.657466988 | 0.667659990 | 0.511622024 |
| 0.720063981 | 0.356463994 | 0.490303997 |
| 0.719987990 | 0.482041997 | 0.496755007 |
| 0.721063991 | 0.607599010 | 0.505891987 |
| 0.695156970 | 0.732534986 | 0.530219977 |
| 0.782544965 | 0.293660021 | 0.487685002 |
| 0.782569994 | 0.419274973 | 0.493518998 |
| 0.782577988 | 0.544580973 | 0.501495000 |
| 0.782661972 | 0.673686961 | 0.514629013 |
| 0.845037988 | 0.356453005 | 0.490864001 |
| 0.845153996 | 0.482021008 | 0.498077997 |
| 0.844049017 | 0.607629999 | 0.508207963 |
| 0.880815026 | 0.732697017 | 0.517417012 |
| 0.907531059 | 0.293651999 | 0.488303977 |
| 0.907561036 | 0.419196980 | 0.495232989 |
| 0.907549997 | 0.545021023 | 0.503933000 |
| 0.907624988 | 0.667593013 | 0.515407976 |
| 0.970048016 | 0.356421000 | 0.492521994 |
| 0.969967030 | 0.481963976 | 0.500674023 |
| 0.971113026 | 0.607490000 | 0.510492968 |
| 0.946443932 | 0.732713006 | 0.518249979 |
| 0.095030000 | 0.232821989 | 0.485588016 |
| 0.220053013 | 0.232813994 | 0.485774009 |
| 0.345075008 | 0.232813005 | 0.485783025 |

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0.470079992        0.232820011        0.485603012
0.595071986        0.232830011        0.485383990
0.720049991        0.232837016        0.485215998
0.845031041        0.232838994        0.485175028
0.970018991        0.232831000        0.485329005
0.846282006        0.762479021        0.516776017
0.594237042        0.761183045        0.541493995
0.317447017        0.827171052        0.514612973
0.257371988        0.830465029        0.498115993
```

TS28
E+ZPE = -1187.29300 eV
1.0
```
    20.0422000885        0.0000000000        0.0000000000
     0.0000000000       34.7140998840        0.0000000000
     0.0000000000        0.0000000000       15.0721998215
```
  B   N   O
 64  64  12
Direct
```
0.022856001        0.250346013        0.502080029
0.022885000        0.376038987        0.499114990
0.023014000        0.501435974        0.493561012
0.023180001        0.628557972        0.489775977
0.085353998        0.313255013        0.501200018
0.085472998        0.438760021        0.497352975
0.085125997        0.564396045        0.490395997
0.089507998        0.689648996        0.495492000
0.147856990        0.250342991        0.502419999
0.147900006        0.375984015        0.500509037
0.147931993        0.501622950        0.495959023
0.148359993        0.625868988        0.484517013
0.210376993        0.313241002        0.502022988
0.210398001        0.438744005        0.500190011
0.210809002        0.564115993        0.496630009
0.207200997        0.689616963        0.500041001
0.272864996        0.250333019        0.502753958
0.272915006        0.375988987        0.501961992
0.272936990        0.501326964        0.501797986
0.272736997        0.627600015        0.502235999
0.335393992        0.313235013        0.502417025
0.335492014        0.438728978        0.502870033
0.335016014        0.564098026        0.506394032
0.337839989        0.688136978        0.499372989
0.397868981        0.250329997        0.502750984
0.397938025        0.375963987        0.502273014
```

| | | |
|---|---|---|
| 0.397980992 | 0.501604984 | 0.505231978 |
| 0.397830986 | 0.625696023 | 0.513288021 |
| 0.460421008 | 0.313236002 | 0.501853003 |
| 0.460430001 | 0.438742000 | 0.502806000 |
| 0.460879996 | 0.564324013 | 0.506932966 |
| 0.455870996 | 0.690396021 | 0.495020009 |
| 0.522875012 | 0.250329997 | 0.502349986 |
| 0.522939964 | 0.376013987 | 0.501016018 |
| 0.522939964 | 0.501413008 | 0.503005028 |
| 0.522691008 | 0.628489017 | 0.502273014 |
| 0.585394016 | 0.313250013 | 0.500767004 |
| 0.585484044 | 0.438800983 | 0.500397992 |
| 0.584878023 | 0.564347969 | 0.500619007 |
| 0.588906997 | 0.688754994 | 0.495395982 |
| 0.647869005 | 0.250347991 | 0.501887012 |
| 0.647908975 | 0.376013987 | 0.499422026 |
| 0.647920014 | 0.501747015 | 0.498764992 |
| 0.647877998 | 0.625567013 | 0.494161986 |
| 0.710387009 | 0.313263007 | 0.500051030 |
| 0.710376969 | 0.438814993 | 0.497869004 |
| 0.710924986 | 0.564360002 | 0.495626994 |
| 0.706551033 | 0.691124036 | 0.495173986 |
| 0.772863997 | 0.250354996 | 0.501739964 |
| 0.772906013 | 0.376045992 | 0.498442992 |
| 0.772926997 | 0.501435974 | 0.495546004 |
| 0.772912008 | 0.628635993 | 0.493675000 |
| 0.835375054 | 0.313268007 | 0.499995001 |
| 0.835468032 | 0.438818015 | 0.496349011 |
| 0.834941951 | 0.564365056 | 0.493231008 |
| 0.839571046 | 0.689020980 | 0.494639007 |
| 0.897860987 | 0.250360985 | 0.501858001 |
| 0.897900006 | 0.376027998 | 0.498355010 |
| 0.897943973 | 0.501748993 | 0.493773011 |
| 0.898164949 | 0.625573002 | 0.493492012 |
| 0.960374995 | 0.313270013 | 0.500445004 |
| 0.960392981 | 0.438821999 | 0.496134987 |
| 0.961046014 | 0.564335991 | 0.491304006 |
| 0.957411030 | 0.690805028 | 0.495198979 |
| 0.022856999 | 0.292266024 | 0.501230010 |
| 0.022907000 | 0.417867982 | 0.497476992 |
| 0.023082000 | 0.543223954 | 0.491452984 |
| 0.023418001 | 0.672015000 | 0.493898989 |
| 0.085371004 | 0.355058020 | 0.500374011 |
| 0.085522003 | 0.480585968 | 0.495229983 |
| 0.084821000 | 0.606329957 | 0.486745008 |
| 0.114755003 | 0.730310998 | 0.521201002 |

| | | |
|---|---|---|
| 0.147861998 | 0.292263002 | 0.501896978 |
| 0.147926997 | 0.417798010 | 0.499351001 |
| 0.147931993 | 0.543527028 | 0.493453004 |
| 0.148688009 | 0.666820987 | 0.480239993 |
| 0.210403997 | 0.355035987 | 0.501618036 |
| 0.210368999 | 0.480578990 | 0.499242993 |
| 0.211255000 | 0.605934961 | 0.493802022 |
| 0.177204999 | 0.728973979 | 0.529343003 |
| 0.272881008 | 0.292250008 | 0.502475964 |
| 0.272942985 | 0.417820016 | 0.501835001 |
| 0.272919003 | 0.543104010 | 0.502090975 |
| 0.272546997 | 0.670851001 | 0.502372037 |
| 0.335417974 | 0.355031015 | 0.502337996 |
| 0.335534006 | 0.480568990 | 0.503811008 |
| 0.334574013 | 0.605943972 | 0.509315000 |
| 0.368235996 | 0.726810979 | 0.467477998 |
| 0.397901005 | 0.292250008 | 0.502408040 |
| 0.397968002 | 0.417784000 | 0.502843015 |
| 0.398018988 | 0.543529995 | 0.507346998 |
| 0.397691995 | 0.666670989 | 0.513783992 |
| 0.460451984 | 0.355037992 | 0.501671028 |
| 0.460420008 | 0.480588990 | 0.504136014 |
| 0.461288975 | 0.606291002 | 0.508885024 |
| 0.432795991 | 0.729306997 | 0.467070990 |
| 0.522907036 | 0.292246986 | 0.501583995 |
| 0.522968989 | 0.417852021 | 0.501379019 |
| 0.522909986 | 0.543232965 | 0.503822018 |
| 0.522594985 | 0.672243020 | 0.497384011 |
| 0.585416951 | 0.355055987 | 0.500209974 |
| 0.585515972 | 0.480668000 | 0.500749003 |
| 0.584291986 | 0.606300013 | 0.498979015 |
| 0.619638015 | 0.731002969 | 0.502556986 |
| 0.647886992 | 0.292265008 | 0.500719011 |
| 0.647925962 | 0.417843999 | 0.499098001 |
| 0.647882995 | 0.543719004 | 0.498209005 |
| 0.647727016 | 0.666315004 | 0.491573995 |
| 0.710407042 | 0.355069998 | 0.499157985 |
| 0.710329005 | 0.480676022 | 0.497243986 |
| 0.711383975 | 0.606262980 | 0.494102002 |
| 0.685217006 | 0.731549007 | 0.501847973 |
| 0.772876035 | 0.292270997 | 0.500451996 |
| 0.772916005 | 0.417892982 | 0.497397994 |
| 0.772919003 | 0.543229998 | 0.494608002 |
| 0.773011029 | 0.672456040 | 0.494271987 |
| 0.835390947 | 0.355073981 | 0.498869994 |
| 0.835505052 | 0.480668989 | 0.495000015 |

| | | |
|---|---|---|
| 0.834444991 | 0.606324023 | 0.493251002 |
| 0.871384965 | 0.731415987 | 0.492544994 |
| 0.897872978 | 0.292278002 | 0.500711988 |
| 0.897917992 | 0.417853999 | 0.496834004 |
| 0.897945971 | 0.543699993 | 0.492502000 |
| 0.898075017 | 0.666315993 | 0.495595990 |
| 0.960390983 | 0.355072003 | 0.499343978 |
| 0.960380990 | 0.480670967 | 0.494239971 |
| 0.961587988 | 0.606189025 | 0.491100993 |
| 0.937034046 | 0.731404998 | 0.493274002 |
| 0.085354998 | 0.231435986 | 0.502528007 |
| 0.210357984 | 0.231427003 | 0.502806000 |
| 0.335370010 | 0.231419998 | 0.502953997 |
| 0.460378992 | 0.231427003 | 0.502870033 |
| 0.585380027 | 0.231434997 | 0.502559011 |
| 0.710364978 | 0.231452992 | 0.502349006 |
| 0.835364015 | 0.231461014 | 0.502349986 |
| 0.960353011 | 0.231447003 | 0.502407028 |
| 0.836935025 | 0.761193979 | 0.489553001 |
| 0.261828998 | 0.749457011 | 0.490101015 |
| 0.584274999 | 0.760321021 | 0.510442032 |
| 0.330445994 | 0.755462994 | 0.439682987 |

C3H8 molecule
E+ZPE = -54.27843 eV
1.0

| | | |
|---|---|---|
| 20.0422000885 | 0.0000000000 | 0.0000000000 |
| 0.0000000000 | 34.7140998840 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 15.0721998215 |

H   C
8   3
Direct

| | | |
|---|---|---|
| 0.934651169 | 0.813067735 | 0.559743658 |
| 0.818291788 | 0.838608847 | 0.546067610 |
| 0.840263954 | 0.879974743 | 0.609151394 |
| 0.875874736 | 0.872686411 | 0.502601753 |
| 0.017953479 | 0.845137077 | 0.659260708 |
| 0.996248722 | 0.876572855 | 0.570733293 |
| 0.961859023 | 0.883965472 | 0.677950503 |
| 0.899974733 | 0.820695404 | 0.665660340 |
| 0.917723690 | 0.835780579 | 0.605709556 |
| 0.859849818 | 0.857868486 | 0.563630120 |
| 0.976678942 | 0.861672458 | 0.629801219 |

O2 molecule
E+ZPE = -9.34683 eV
1.0
   20.0422000885     0.0000000000     0.0000000000
    0.0000000000   34.7140998840     0.0000000000
    0.0000000000     0.0000000000   15.0721998215
  O
  2
Direct
  0.270345460    0.753191808    0.479518673
  0.324684558    0.757858134    0.442511323


C3H6 molecule
E+ZPE = -46.56043 eV
1.0
   20.0422000885     0.0000000000     0.0000000000
    0.0000000000   34.7140998840     0.0000000000
    0.0000000000     0.0000000000   15.0721998215
  H   C
  6   3
Direct
  0.750351141    0.864783525    0.578013441
  0.863637925    0.838967360    0.522622510
  0.863934464    0.875307868    0.438933890
  0.870653800    0.887825542    0.553438810
  0.676806560    0.881050721    0.454943409
  0.749814163    0.886070890    0.379335350
  0.771844286    0.870872693    0.512580558
  0.846184175    0.868213380    0.505991864
  0.730783645    0.879778097    0.445800165


H2O molecule
E+ZPE = -13.65064 eV
1.0
   20.0422000885     0.0000000000     0.0000000000
    0.0000000000   34.7140998840     0.0000000000
    0.0000000000     0.0000000000   15.0721998215
  O   H
  1   2
Direct

          0.245814881        0.724484904        0.419714778
          0.289850812        0.734947269        0.432194510
          0.217404311        0.747017860        0.413030731


C3H7 radical
E+ZPE = -49.28 eV
1.0
        20.0422000885        0.0000000000        0.0000000000
         0.0000000000       35.0000000000        0.0000000000
         0.0000000000        0.0000000000       15.0000000000
     H   C
     7   3
Direct
        0.415921234        0.549724470        0.534209379
        0.421961793        0.556507492        0.370552667
        0.464068745        0.599494171        0.398137728
        0.510932504        0.557998548        0.374630578
        0.518398945        0.548230362        0.625382932
        0.569070512        0.553307343        0.528243319
        0.531079994        0.593828964        0.576535670
        0.463528055        0.557145800        0.503324572
        0.464834884        0.568013491        0.407572397
        0.522823527        0.563139398        0.561130651


NO molecule
E+ZPE = -12.13 eV
     1.00000000000000
     20.0422000884999996    0.0000000000000000    0.0000000000000000
      0.0000000000000000   34.7140998839999995    0.0000000000000000
      0.0000000000000000    0.0000000000000000   15.0721998214999999
     N   O
     1   1
Direct
   0.1228198913309192  0.7333676986779997  0.5486026647547830
   0.0938901076690833  0.7607023073220015  0.5730472842452188


N2O molecule
E+ZPE = -21.09 eV
     1.00000000000000
     20.0422000884999996    0.0000000000000000    0.0000000000000000
      0.0000000000000000   34.7140998839999995    0.0000000000000000
      0.0000000000000000    0.0000000000000000   15.0721998214999999

```
  N   O
   2   1
Direct
  0.3921045636028233  0.7875684579799869  0.5105618312732034
  0.4429200841547661  0.7724720295455126  0.5132854094107007
  0.3389153752424108  0.8033695354745005  0.5077127473160936
```

N2 molecule
E+ZPE = -16.44 eV

```
   1.00000000000000
    20.0422000884999996    0.0000000000000000    0.0000000000000000
     0.0000000000000000   34.7140998839999995    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0721998214999999
   N
    2
Direct
  0.1307720805234383  0.7797906962384547  0.5191661911361920
  0.1865179234765619  0.7799492977615499  0.5195538208638069
```

OOH radical
E+ZPE = -12.88 eV

```
   1.00000000000000
    20.0422000884999996    0.0000000000000000    0.0000000000000000
     0.0000000000000000   34.7140998839999995    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0721998214999999
   O   H
    2   1
Direct
  0.2656930010504726  0.8208331921420247  0.5311145086542897
  0.3302786991649618  0.8110443062281584  0.5216110365287356
  0.2403182857845628  0.7992425466298171  0.5043044918169790
```

Atomic coordinates of relaxed structures involved in B loss from BNNR12O:

B2O3 bulk unit cell
E+ZPE = -120.68 eV

```
   1.00000000000000
     4.3944001197814941    0.0000000000000000    0.0000000000000000
    -2.1972000603195361    3.8056621378765922    0.0000000000000000
     0.0000000000000000    0.0000000000000000    8.6466999053955078
   B   O
    6   9
```

Selective dynamics
Direct
 0.5989367161477374  0.8219824307581413  0.1090097092203146  T  T  T
 0.4010618873921577  0.2230672530634729  0.2243314785233730  T  T  T
 0.1779986960423137  0.7769378330647664  0.4423502861008349  T  T  T
 0.7769409438010915  0.1779976258636274  0.5576502207146462  T  T  T
 0.2230683739969520  0.4010595320681190  0.7756704944028769  T  T  T
 0.8219827780289488  0.5989338253981988  0.8909924457244845  T  T  T
 0.8289064811397665  0.8289066518786665  0.0000010571132590  T  T  T
 0.5932221292389064  0.1312345403420593  0.1289395963697120  T  T  T
 0.4068027544938578  0.5380307922753812  0.2043988738590747  T  T  T
 0.1710623055313159 -0.0000025823162706  0.3333319372564778  T  T  T
 0.8687467986412962  0.4620068953960754  0.4623006043884464  T  T  T
 0.4620118233125677  0.8687472220525131  0.5376997480956126  T  T  T
-0.0000023418128987  0.1710623456318590  0.6666692878665637  T  T  T
 0.5380349085184314  0.4068044317961487  0.7956016832668046  T  T  T
 0.1312357455275523  0.5932212027272452  0.8710625770975154  T  T  T


BO (one dimentional)
E+ZPE = -104.93 eV
   1.00000000000000
   20.0422000884999996    0.0000000000000000    0.0000000000000000
    0.0000000000000000   34.7140998839999995    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721998214999999
   B   O
   8   8
Direct
 0.0213562207302829  0.2493087639723583  0.5044955028476821
 0.1463503321680832  0.2493254007206929  0.5048806272689745
 0.2713416922017515  0.2493286131074299  0.5053641594537410
 0.3963277534490430  0.2493159578662443  0.5055721972825324
 0.5213267238709918  0.2492991924876833  0.5053741622611554
 0.6463295957672273  0.2492796509892656  0.5048998760320771
 0.7713478436024701  0.2492809221816685  0.5045146196823680
 0.8963600261787761  0.2492876377647946  0.5043466592038186
 0.0838621390469712  0.2312518498198415  0.5052191368758585
 0.2088455298482259  0.2312622454419895  0.5054607669200166
 0.3338278886743069  0.2312521977615347  0.5056434922302699
 0.4588157736758376  0.2312424831311048  0.5056524914585552
 0.5838203244692224  0.2312219355737497  0.5054520230112303
 0.7088426428740249  0.2312196852965940  0.5052191851986976
 0.8338580424606690  0.2312208090287982  0.5050584356601391
 0.9588675659821178  0.2312327098562363  0.5050766046128956

12O-B2O3
E+ZPE = -1040.48 eV
  1.00000000000000
    20.0422000884999996    0.0000000000000000    0.0000000000000000
     0.0000000000000000   34.7140998839999995    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0721998214999999
  B   N   O
   56   64    4
Direct
 0.3313577525469808  0.6911067602181410  0.4792202887198159
 0.4488944269588368  0.6932027207677511  0.4786589287631186
 0.6400602197684259  0.6277061326156750  0.4831167893839952
 0.5813354559647124  0.6910259954610123  0.4792179005078046
 0.1988674850099642  0.6932617557686475  0.4792176532002675
 0.0813225448069853  0.6910994007949082  0.4786426940020178
 0.6988552607869846  0.6931714478696986  0.4784194145381423
 0.8312977451349362  0.6910114519004087  0.4780730137970901
 0.7649322200476760  0.6306491727057655  0.4822661212472683
 0.9488239804989740  0.6932099148418174  0.4779898233807463
 0.1400467641659504  0.6278007078789161  0.4846923744286454
 0.8900519996213845  0.6277369122434754  0.4836622844887188
 0.0149300682966470  0.6307186296134056  0.4836062478877236
 0.7029833001189548  0.5664516734251837  0.4859869702191036
 0.5149494806238596  0.6307202383582625  0.4858341990836208
 0.8269631831103808  0.5664646095984990  0.4849970348333461
 0.2649408013185361  0.6307952481931013  0.4869824616630709
 0.9529754914970101  0.5664915448504527  0.4868617563543622
 0.5769632913901591  0.5665323290884612  0.4899964155459909
 0.0769491825320859  0.5665786234250947  0.4905489889063160
 0.7649602137666595  0.5035316613680563  0.4858493970589640
 0.8899642214352180  0.5038550663806258  0.4866111984554026
 0.6399516996378282  0.5039151600134876  0.4911855354687832
 0.2029669923655669  0.5666616010218299  0.4945894144073810
 0.0149598039722535  0.5036403963970029  0.4926206731057832
 0.8275065306938499  0.4408843754850487  0.4828294547249235
 0.3900630155907354  0.6278712712009379  0.4887416531382120
 0.7023226835489781  0.4409721788405374  0.4872845156150595
 0.9524915988683288  0.4409854541738881  0.4890863945605444
 0.4529885924702066  0.5666357876583975  0.4948660568693529
 0.1399461937381290  0.5041091251345754  0.5006466383553300
 0.7646330717594315  0.3781453466929165  0.4766376879262001
 0.5149863881557727  0.5037580521284752  0.4996725625875592
 0.8903471350978425  0.3781159916479052  0.4779953437649407
 0.3269615857755927  0.5667081345379834  0.4967658856586098

0.5774877213085067 0.4411442697262083 0.5002745622399736
0.0774864617786162 0.4411862066076999 0.5023295448468000
0.8275761890978736 0.3148418003849961 0.4625673544760407
0.6397058398968066 0.3783174633685240 0.4924453974917400
0.0151686378014470 0.3783646911089713 0.4954223581590400
0.7005239688260899 0.3147419119730094 0.4711987992848034
0.9544842010810912 0.3147226926057080 0.4739458016070072
0.2649646531006943 0.5039242734119094 0.5064131508978089
0.0775195903519963 0.3152236457204176 0.5132614451299903
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Atomic coordinates of Relaxed structures of different possible configurations after first C-H cleavage of C3H8 on different sites of BNNR14O edges:

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    0.0000000000000000    0.0000000000000000   15.0721998214999999
   B   N   O   H
   64   64   14   1
Direct
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0.0894643150173922 0.3151946614288448 0.4990774984452878
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    B   N   O   C   H
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  0.0205141253278427  0.6294203270073240  0.4927414151413601
  0.0834455895373125  0.3151310280717752  0.4878848132940732
  0.0834540439897040  0.4402102488967259  0.4923166673779988
  0.0828140434541496  0.5654645849037436  0.4911521382558632
  0.0861882647424892  0.6903772853981351  0.4951239432774699
  0.1448916308462884  0.2522018993062218  0.4865949311611644
  0.1458012532339055  0.3776565668865715  0.4892680958184243
  0.1459372106483485  0.5029231484082786  0.4917762856997214
  0.1457853513433918  0.6268161516291144  0.4856852559887770
  0.2075115518627442  0.3150078859693792  0.4876589183366349
  0.2084382257953834  0.4401121454119945  0.4907405158686160
  0.2089467729302754  0.5653040004945922  0.4922510305509817
  0.2052452692021518  0.6902410450531846  0.4943590830813207
  0.2675618647788198  0.2520131401860866  0.4911250245238534
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P5
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    0.0000000000000000   34.7140998839999995    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721998214999999
   B   N   O   H
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 0.0829817889867615  0.4391193839083872  0.4962206435582179
 0.0823708142040122  0.5643578543411596  0.4915751587106550
 0.0854880114930790  0.6892745179522758  0.4940769118473540
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0.7204042057740949  0.6072492099739009  0.4902869864749846
0.6950084279581290  0.7306729792405946  0.5087927699548018
0.7817231065763579  0.2933916255282440  0.5043916435773497
0.7816960697291151  0.4189727780003096  0.5030616942038293
0.7817515767358856  0.5442018388959937  0.4969193192518802
0.7828910257322050  0.6727519863605238  0.4906862455918883
0.8442167657942363  0.3561429815644104  0.5038177761072333
0.8443071478394444  0.4816397477396350  0.5004515050701670
0.8436043379207021  0.6069917715314261  0.4947717490305266
0.8788974098806364  0.7314795710633533  0.4806336417217736
0.9067519440436271  0.2933544525944498  0.5040063717972600
0.9067434585352814  0.4188469322735529  0.5025871489787832
0.9068541909989492  0.5444938552660616  0.4974377555400125
0.9071847089503251  0.6669908881853672  0.4966418151304808
0.9692835572729592  0.3561072037183521  0.5036971996825272
0.9692325303595126  0.4815542800652821  0.5002459362143981
0.9704386680004902  0.6069161671229679  0.4950059162504701
0.9445298021065867  0.7319891859847871  0.4804002075686711
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0.2193530136172086  0.2325738075184702  0.5047389541405920
0.3443385930411864  0.2326058023178419  0.5048319877707783
0.4692939044610682  0.2326248342471544  0.5046951038664176
0.5942349785437173  0.2326221186377140  0.5045317027775127
0.7192091024514369  0.2325921308453545  0.5043359318337082
0.8442309614181767  0.2325503296363465  0.5042533375342444
0.9692676189203908  0.2325305536399043  0.5043373374538120
0.8436817769596914  0.7608652164955956  0.4713340494562814
0.4727613868160461  0.7571637155162634  0.4110365093384800
0.2258415125110247  0.7598813433718163  0.5281548315305642
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0.3381896974938670  0.7515125263917355  0.4000448979291775
0.0919970604599669  0.7613521051136161  0.5267337080986465
0.4539220933019408  0.7976212851374811  0.4373648864612392
0.4468237559033810  0.8022423015591045  0.5368323769508123
0.5082037286990229  0.8218668747175002  0.3952329184861156
0.4057945469336346  0.8032461832695219  0.4050673307325283
0.4053078360602100  0.7850347047109807  0.5632415207655441
0.4929225405327173  0.7945717046111724  0.5719508554396953
0.4350885200261203  0.8326065174790642  0.5507735892924259
0.5127103024257593  0.8154553751197255  0.3240895361436102
0.4949869122168806  0.8524662203010891  0.4020484688178030
0.5567674745074740  0.8169101542590198  0.4269675030025226
0.6344862825822588  0.7795047437251199  0.5440719074667726

P7
E+ZPE = -1256.56 eV
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    0.0000000000000000  34.7141000000000020   0.0000000000000000
    0.0000000000000000   0.0000000000000000  15.0722000000000005
   B   N   O   C   H
   64   64   14   3   8
Direct
 0.0310020703809855  0.2519860081486058  0.5031776299966637
 0.0309908157529790  0.3776380164060313  0.5010581828113700
 0.0309814316973984  0.5029432282844368  0.5012621848603445
 0.0306964777093555  0.6300179029659887  0.5079337548501499
 0.0934884649950618  0.3149087394706598  0.5025307149861575
 0.0935464850160557  0.4403956754686007  0.5013491565901802
 0.0928869333087761  0.5658851433816494  0.5027858182281051
 0.0964814850434124  0.6907985768849869  0.5135708144834510
 0.1560171218822077  0.2520165900287452  0.5032298422356831
 0.1560031573474774  0.3776739519267593  0.5023895904885478
 0.1559777542169911  0.5033325323708056  0.5022500239406256
 0.1556867654752097  0.6271983474844944  0.5019418567144029
 0.2184927525345444  0.3149427705110455  0.5028831257743533
 0.2184908637869327  0.4404975144048109  0.5028300417476004
 0.2188983203319879  0.5659327365260722  0.5039193398708974
 0.2155514226831485  0.6903128409059320  0.5104929477096718
 0.2810114650598123  0.2520450634319502  0.5029832874420066
 0.2809971937820706  0.3777489206520031  0.5027515479992815
 0.2810869663054447  0.5032068194655537  0.5043761625316989
 0.2808749324028668  0.6298588748510952  0.5075226743779027
 0.3434735754472200  0.3149751582131657  0.5022815645928702
 0.3435639925209699  0.4405505329882686  0.5033144225740429
 0.3432185803492160  0.5662691387064669  0.5082442158256057
 0.347098365149466   0.6910294720175116  0.5010815735925078
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0.5934175375069373  0.3149518591111473  0.5001537251706267
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0.5930286419304664  0.5660415640904262  0.4994296475872773
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0.6559165563525937  0.3776720007769114  0.4984306017687459
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0.8435073687888490  0.4403352762314086  0.4983303389345295
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0.9689247091848898  0.5657822808957391  0.5039650861728973
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0.0310061743905550  0.4194571146402168  0.5005980776020280
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0.1560012411469103  0.2939261719769064  0.5029980504920673
0.1560298908969386  0.4194855534869788  0.5022071379143682
0.1558867288982739  0.5452602831389797  0.5024119276365440
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0.7810649647494614  0.6734174204019041  0.5125107326864153
0.8434416089831487  0.3566571055586607  0.4994983165299232
0.8435510793243637  0.4821674592600544  0.4985251936260227
0.8424814569841459  0.6076380974307583  0.5062637908229846
0.8777672206104512  0.7324388783304485  0.5083900958033354
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0.9059774741378916  0.4193874435249754  0.4990907987253834
0.9059473825193649  0.5451418604109151  0.5020925878308304
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0.9684953767075868  0.3566606194511195  0.5006364634024081
0.9684118927283762  0.4821740835329891  0.5002866202583718
0.9693547601384509  0.6076445194313180  0.5079356288571830

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0.4684568743834845  0.2331395028179912  0.5026512017681100
0.5934212245181172  0.2331214378112918  0.5026789585413454
0.7184015690631753  0.2331077592418183  0.5030051917847160
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0.5925062957499563  0.7554818092258628  0.5802813666456075
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0.0925643849730946  0.7621656568174160  0.5483132747491695
0.4751012620434736  0.7911115751487472  0.4129271290877199
0.5470236082845403  0.8049140919773095  0.4130563264474958
0.4376730218237128  0.8044786518493510  0.3306708719174054
0.4490971269181472  0.7999784415472675  0.4737542478078112
0.5726310947982256  0.7977003125638973  0.4751241653553748
0.5745518195329922  0.7921712783820993  0.3570490490962328
0.5482081833882120  0.8364010056635678  0.4047375770472854
0.3861096408920588  0.7939575948383890  0.3303934511284012
0.4367460528230893  0.8361683918148017  0.3286370823106495
0.4632188989823902  0.7943544421563757  0.2703527357113771
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P8
E+ZPE = -1256.35 eV
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    0.0000000000000000   34.7141000000000020    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0722000000000005
   B   N   O   H   C
   64   64   14   8   3
Direct
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 0.0409620602150724  0.5029263045507122  0.4917097306074893
 0.0406226693567007  0.6295587890048040  0.4904223006154425
 0.1034543876111442  0.3148834082384582  0.4982540937397957
 0.1035058067731427  0.4403956390768471  0.4962643232088624
 0.1030781088507879  0.5659249270364199  0.4919383242015769
 0.1055766746513527  0.6907468804744994  0.5021042783427774
 0.1659688246225102  0.2519850122876832  0.4983391456016406

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0.2283938618170609  0.4404789475001536  0.5003841391982888
0.2289026974575279  0.5661414490716652  0.5002679228337925
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0.2909178222244577  0.3776969010598421  0.5008771153422700
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0.3534255671650968  0.3149069548714039  0.4998719315955213
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0.5410205065152383  0.6296171346044162  0.5019314120036924
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0.2518771345798285  0.7921431402066119  0.5664753364215187
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P9
E+ZPE = -1256.04 eV
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   B   N   O   C   H
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P10
E+ZPE = -1257.19 eV
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    0.0000000000000000    0.0000000000000000   15.0722000000000005
   B   N   O   H   C
   64   64   14   8   3
Direct
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0.0911514385149088  0.5655155735422890  0.4893116992484319
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0.1540906725645381  0.3771859850058755  0.4937887819586451
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0.5834474738875599  0.7602635794499832  0.5496354921337598
0.3381022385704071  0.7591039334562026  0.4550541283282001
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0.6211924815637460  0.7960828992249631  0.5686853302175692
0.6410833201747579  0.8160172030589123  0.4829959275799425
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0.6659093403882252  0.7869405437432206  0.6052989105034214
0.6742250315453617  0.7976723968419606  0.4433525717109887
0.5969048595269015  0.8239581830953995  0.4436450873740512
0.6685367125071480  0.8425615058568994  0.4990594224978153
0.5614246259561995  0.8036664679179566  0.6878130081250262
0.5992754200145782  0.8463674220442101  0.6458010133610301
0.5281134838142236  0.8269458937202572  0.5916255623312026
0.5116358752653554  0.7627603581146190  0.4916267922966071
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P12
E+ZPE = -1257.18 eV
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    0.0000000000000000   34.7141000000000020    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0722000000000005
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 0.0278294012871498  0.5034320935659551  0.4972159723799194
 0.0279190398123248  0.6301792418254593  0.4931888949724055
 0.0903037087101950  0.3153185858028706  0.4984409039381603
 0.0903395985700755  0.4407899119999712  0.4974741051641871
 0.0898883703490299  0.5662587624831232  0.4924560385187533
 0.0933535025788075  0.6910770218881339  0.4933998157123369
 0.1528293074906131  0.2524230645314702  0.4982887049470790
 0.1528171655106547  0.3780271386378047  0.4980092269095309
 0.1527876897235103  0.5036303268441458  0.4953276103958828
 0.1528184484930719  0.6276907657412067  0.4843775579577212
 0.2153513987884850  0.3153075346354228  0.4983789639348686
 0.2152612770993443  0.4407601789154612  0.4975834486461537
 0.2156851172018364  0.5662191089441606  0.4937320878269702
 0.2118076398587689  0.6912009044141740  0.4958083173340668
 0.2778767823084678  0.2524428877503127  0.4982627716504737
 0.2778454008719535  0.3780606290856738  0.4985910886417599
 0.2777346591888872  0.5033543710959876  0.4984929011486301
 0.2776381253377096  0.6300217326813851  0.4959715206761643
 0.3403784368843361  0.3153528228784879  0.4986829433090705
 0.3403495828068799  0.4407993143774362  0.4998428050659456
 0.3396661770555340  0.5661609515340587  0.5019936543492918
 0.3436215906777846  0.6910017008029357  0.4938401768082770
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 0.4023148648779937  0.6275626334583038  0.5091984449253673
 0.4653903643350574  0.3154223101532381  0.4989522793245271
 0.4653430511439254  0.4409248811413633  0.5014901854382288
 0.4655628983227516  0.5662612311402810  0.5051968752742582
 0.4620290266789766  0.6905053910854804  0.4976126430416770
 0.5278720791467464  0.2525366108954969  0.4981085897117055
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 0.5278792137214197  0.5036503101351144  0.5027184052680411
 0.5274177079470590  0.6300694451599895  0.5026082346927865
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0.8447970546612424  0.6905876173926728  0.4893534637652763
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0.9658635408662306  0.5663200851663319  0.4989015849045444
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0.7380388007084377  0.8006054953656800  0.6660163163517652
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P13
E+ZPE = -1256.46 eV
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     0.0000000000000000    0.0000000000000000   15.0722000000000005
   B   N   O   C   H
   64   64   14   3   8
Direct
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 0.0894371017028206  0.4410582031145438  0.5002300300817666
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 0.1519408818608099  0.5038666898858182  0.5006414585803398
 0.1521440916445940  0.6277134181895505  0.4892960119678804
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0.4644325159182330 0.4410539141042236 0.5030365430437556
0.4647521549825271 0.5665029267672281 0.5064730227146015
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P15
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    0.0000000000000000  34.7141000000000020   0.0000000000000000
    0.0000000000000000   0.0000000000000000  15.0722000000000005
  B   N   O   C   H
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 0.0184820381676829  0.5030964048811839  0.4946531070081335
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 0.0808990215022476  0.3149787787643916  0.4993013366171652
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0.9498234754692305  0.8007418761660503  0.5439181798578474
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0.8928269351543037  0.8288286836207135  0.3594249819072601
0.9297921511435447  0.7828820870966595  0.3777610700943228
0.7012841866449619  0.7563003924810872  0.5258445725156307
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Atomic coordinates of Relaxed structures with SCAN+rvv10 functional:

C3H8 molecule
E+ZPE = -56.77 eV
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    0.0000000000000000  34.7140998839999995   0.0000000000000000
    0.0000000000000000   0.0000000000000000  15.0721998214999999
  H   C
   8   3
Direct
 0.9344134494529629  0.8133566362785397  0.5599642487604299
 0.8178068641523132  0.8389231421370177  0.5455382594460834
 0.8401731871966656  0.8799980654928449  0.6082801942013472
 0.8759851687080599  0.8725611502624094  0.5026062477561095
 0.0169494154031543  0.8458653454409442  0.6594082729640897
 0.9950593711752292  0.8767519422773283  0.5707352657177066
 0.9599941247150277  0.8841722273138831  0.6768748431178870
 0.8991953301629489  0.8210296010757552  0.6650492280799970
 0.9171299442775978  0.8359055808898921  0.6054495240369554
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0.8594697730462617  0.8579346842574305  0.5631175021962739
0.9756235187097647  0.8620115565739536  0.6295463627231207

O2 molecule
E+ZPE = -11.86 eV
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   19.9165000885000012    0.0000000000000000    0.0000000000000000
    0.0000000000000000   34.7140998839999995    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721998214999999
  O
   2
Direct
  0.3132380951563819  0.8412382739318209  0.4818638513541124
  0.2516945382961678  0.8407668096269711  0.4795648533593998

C3H6 molecule
E+ZPE = -48.89 eV
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   19.9165000885000012    0.0000000000000000    0.0000000000000000
    0.0000000000000000   34.7140998839999995    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721998214999999
   H    C
   6    3
Direct
  0.8160234222436725  0.8501569694176618  0.5273851583599997
  0.8397506096961124  0.9177343596434414  0.4683084464358894
  0.7520867608559988  0.9264502568565773  0.4628193201905285
  0.7928327220868620  0.9207259139979013  0.5665891016285561
  0.7203455850914322  0.8205382442568329  0.4553576972478933
  0.6884297530565153  0.8684846936796541  0.4220926754905106
  0.7788163617647327  0.8681943380233117  0.4945775505650816
  0.7911592542076266  0.9104753783840187  0.4979011540089776
  0.7267055309970448  0.8515398587405995  0.4554489900725613

H2O molecule
E+ZPE = -14.77 eV
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   19.9165000885000012    0.0000000000000000    0.0000000000000000
    0.0000000000000000   34.7140998839999995    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721998214999999

O   H
1   2
Direct
0.8337152645730488  0.8161097564613149  0.4634337043564931
0.8778612809468911  0.8270963472665599  0.4699487503074650
0.8391034444800591  0.7891739282721298  0.4770475363360427




IM0 (14O)
E+ZPE = -1330.55 eV
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    0.0000000000000000   34.7140998839999995    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721998214999999
  B   N   O
  64   64   14
Direct
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 0.0214089064574685  0.3763093252865117  0.4996088411729646
 0.0214694660214103  0.5008119972347975  0.4948120279581210
 0.0209818146159104  0.6267276260107120  0.4910431711164923
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 0.0839765339704758  0.4386871328951890  0.4980514273957387
 0.0833974781902195  0.5633717315451555  0.4919780220506731
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 0.1463650667234785  0.2513899613956166  0.5047209720391292
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0.7729861361141667  0.5430014702159301  0.4946540864576502
0.7731670399066358  0.6715466043364329  0.4941973308341128
0.8351269641236482  0.3556141403810879  0.5001795296181555
0.8354643297505167  0.4806903618549056  0.4975086951563191
0.8345946461301945  0.6059416331843671  0.4961424703479960
0.8706422866062431  0.7295752274005638  0.4825889174059753
0.8975895852077252  0.2930782286686737  0.5001351936573925
0.8977940574754049  0.4180964641375111  0.4993511813595431
0.8980310333511280  0.5434902443372085  0.4963006459834102
0.8981072241427553  0.6657169475741257  0.5033098834006533
0.9602410038883897  0.3556296522153650  0.5002353601103555
0.9604038262974055  0.4807331142952793  0.4974658631633359
0.9615908730004771  0.6058513499590451  0.4968224252794061
0.9362750179529906  0.7300536671012723  0.4832368307669822
0.0851135419086918  0.2327421358090186  0.5002769119773800
0.2101029571706091  0.2327326408235879  0.5003426363788491
0.3350593856460121  0.2327252143482758  0.5004072586013648
0.4600968432778825  0.2327184294112991  0.5003880367206601
0.5851026354668781  0.2327182283652205  0.5002380058365947
0.7101241974775014  0.2327037214695656  0.5000805800595765
0.8351036088548147  0.2327231376664229  0.4999718751635407
0.9601309586846012  0.2327367855405564  0.5000269825561242
0.8355358425553854  0.7584902935567577  0.4695108912754673
0.4666536582480549  0.7534509149450437  0.4257316158764977
0.2601246141205736  0.7504570452106325  0.4866953720462063
0.5831093316484101  0.7543557924099884  0.5469960635375115
0.3343646586013062  0.7571685606974980  0.4365950724038922
0.0820667230149646  0.7570338092878930  0.5381224115321753

Atomic coordinates of Relaxed structures with PBE-D3 functional:

C3H8 molecule
E+ZPE = -54.34 eV
  1.00000000000000
  20.0422000884999996    0.0000000000000000    0.0000000000000000
   0.0000000000000000   34.7140998839999995    0.0000000000000000
   0.0000000000000000    0.0000000000000000   15.0721998214999999
  H   C
   8    3

Direct
 0.9346652605382714  0.8130448740256100  0.5597249132830212
 0.8182722329890072  0.8386162763034383  0.5460694719682256
 0.8402850386730776  0.8799834443355770  0.6091679372279258
 0.8758741636031975  0.8726884693558851  0.5025984630175115
 0.0179523167063946  0.8451426294011575  0.6592747400320237
 0.9962479511000124  0.8765741785365954  0.5707345789538575
 0.9618379109272582  0.8839723958326854  0.6779410447916541
 0.8999810800423298  0.8206890675028028  0.6656647498994557
 0.9177330257730916  0.8357666994238010  0.6056971140717063
 0.8598355981545014  0.8578727010301782  0.5636272132029629
 0.9766854644928585  0.8616792752522722  0.6298096725516390

O2 molecule
E+ZPE = -9.35 eV
   1.00000000000000
    20.0422000884999996    0.0000000000000000    0.0000000000000000
     0.0000000000000000   34.7140998839999995    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0721998214999999
   O
    2
Direct
 0.2703454361455613  0.7531918492819258  0.4795186668642302
 0.3246845578544395  0.7578581477180748  0.4425113291357690

C3H6 molecule
E+ZPE = -46.58 eV
   1.00000000000000
    20.0422000884999996    0.0000000000000000    0.0000000000000000
     0.0000000000000000   34.7140998839999995    0.0000000000000000
     0.0000000000000000    0.0000000000000000   15.0721998214999999
   H    C
    6    3
Direct
 0.7503260221570035  0.8647631529416647  0.5780215207022613
 0.8637072195861930  0.8389530264138028  0.5226451378020993
 0.8639376636161877  0.8752957475315403  0.4389122507722157
 0.8706251265364697  0.8878716930392572  0.5534112442007266
 0.6767853426623675  0.8811005591972140  0.4549216277808694
 0.7498225938278200  0.8860720661589988  0.3793634042182654
 0.7718293536368194  0.8708391231183845  0.5125723784544801
 0.8462060273404803  0.8682007490416813  0.5059987067527882

 0.7307707156366662  0.8797739565574656  0.4458136323162981

H2O molecule
E+ZPE = -13.66 eV
  1.00000000000000
   20.0422000884999996    0.0000000000000000    0.0000000000000000
    0.0000000000000000   34.7140998839999995    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721998214999999
  O   H
   1    2
Direct
 0.2458148917750691  0.7244849248071361  0.4197147879488909
 0.2898508107430047  0.7349472437574534  0.4321945005049344
 0.2174043024819170  0.7470178644354064  0.4130307315461792

IM0 (14O)
E+ZPE = -13.66 eV
  1.00000000000000
   20.0422000884999996    0.0000000000000000    0.0000000000000000
    0.0000000000000000   34.7140998839999995    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721998214999999
  B   N   O
   64   64   14
Direct
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 0.0213499653660728  0.3754404973565035  0.4999617374248556
 0.0213640199323006  0.5007787547808671  0.4949353563741962
 0.0211344207959136  0.6278037450840311  0.4909208500542281
 0.0838452207618502  0.3127092873521752  0.5026842078080561
 0.0838934062217364  0.4381964444188011  0.4982608401269897
 0.0833379831275719  0.5637475475537691  0.4917896393606457
 0.0867469177241036  0.6887296133391761  0.4929856488955854
 0.1463481919870826  0.2498139914555418  0.5048619323393758
 0.1463452599081864  0.3754490434203245  0.5015170335151981
 0.1463292938705482  0.5011265617841899  0.4966665201164084
 0.1462725591599423  0.6251507082079161  0.4852935362762648
 0.2088398816977921  0.3127252119251814  0.5039503553610586
 0.2087916533697856  0.4382461526746460  0.5009757341482948
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 0.2713229482048735  0.3754858104118865  0.5036498378873729

0.2713202806288060 0.5008850252614973 0.5013341351087405
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0.3334118078431463 0.5637724096409515 0.5032336351903950
0.3373034217162522 0.6882609407953734 0.4866829550823553
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0.3964371460796228 0.6253979923307664 0.5072178658148948
0.4588226764633485 0.3127023949848265 0.5050194204984760
0.4587631939566041 0.4381915674196474 0.5038029843481261
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0.5213154708088963 0.2497874795844923 0.5053529797982200
0.5213113476459084 0.3754312591882580 0.5036780367890834
0.5212884175897475 0.5007657065595273 0.5011240241363337
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0.9593047651084563 0.5635989343809406 0.4932622629099143
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0.9588648079870976  0.2308932080904975  0.5050815653436233
0.8332598337471093  0.7588329950130477  0.4627841425466179
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0.0801043557900122  0.7588068415332084  0.5345514591762776


TS1
E+ZPE = -1259.75 eV
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    0.0000000000000000   34.7140999355556019    0.0000000000000000
    0.0000000000000000    0.0000000000000000   15.0721999008333007
   B   N   O   H   C
   64   64   14   8   3
Direct
  0.0153682781926404  0.2537825713895754  0.5077638626101875
  0.0153577584531787  0.3794079889016984  0.5059521725678062

0.0153278808341956 0.5046572738623366 0.4987393405757558
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0.0778872436312039 0.4421265812874645 0.5050610044438483
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0.0808728851250875 0.6921071656904955 0.4760500911485651
0.1403646184510849 0.2538019845711024 0.5084849126955570
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0.3278424594795840 0.3167038156275539 0.5104049982658262
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0.3905841041472061  0.6702780344834947  0.4940602756072042
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0.5155448951125597  0.6743682420570442  0.4775519365550450
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0.7027696494727997  0.4838170515123219  0.4973643656031314
0.7036375508205736  0.6089830324043087  0.4785387885265702
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0.8902673040464057  0.5468380759687419  0.4911192883693647
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0.9528757599720038  0.3584400076887854  0.5054779600515372
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0.9528796269888518  0.2348531889052759  0.5077717814033458
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0.8925866107433613  0.7862934739269560  0.6084972763826424
0.9822310475759800  0.7485854896579111  0.6867937674107890
0.0454921761969551  0.7772203519741745  0.6342470607787939
0.9923736191421575  0.7975753282953173  0.7160825648904727
0.9261242564784741  0.8261878917572713  0.4771551691906624
0.9517460370088180  0.8507732902778889  0.5743390724251172
0.0118454695040077  0.8246791293563662  0.5114096055435188
0.9452425047564689  0.7895641079640556  0.5898498715918152
0.9940067146522997  0.7771955143406168  0.6593279127132964
0.9598637815911248  0.8242397317836196  0.5345797555473673
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    0.0000000000000000   34.7140998839999995    0.0000000000000000
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  B   N   O
  64   64   12
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 0.0323058797225116  0.5033617172330125  0.5026786592282106
 0.0322463885024826  0.6305052083611373  0.5024486519360519
 0.0948173132376940  0.3152081444635456  0.4994608686323286
 0.0948461645181241  0.4407349127317604  0.5026284738164351
 0.0942842224756002  0.5662946732096368  0.5032374481256968
 0.0985922969410963  0.6908855512455520  0.5010829926037728
 0.1573239270488589  0.2523095931525247  0.4975112602371748
 0.1573065140855392  0.3779503319685202  0.5016714740202460
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 0.1573873658024900  0.6275505100608516  0.5015446180785397
 0.2198228574038357  0.3152060172360661  0.4998417220602974
 0.2197573076624838  0.4407364497807170  0.5031006625816745
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 0.2823110874134464  0.3779773076841878  0.5014018950916463
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0.4698268682598802 0.3152101168528896 0.4976505953956237
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TS15'
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  B   N   O
   64   64   14
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 0.0854629509569682  0.4388689434879545  0.4984471244274523
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0.1479141405966864  0.5018103129085869  0.4978405535232301
0.1479970356965607  0.6258105810311220  0.4882404558652945
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0.2103567893505973  0.4389281120894398  0.5009960715115520
0.2108594585068360  0.5644549997241967  0.4981392713213831
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