THE LOWER ELECTRONIC STATES OF MoN

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We find that the ground state of MoN(4Σ−) has a covalent triple bond where the σ bond is dπ-like on the Mo, leading to a quartet state with unpaired electrons in the Mo 5s, Mo 4dδ,1, and Mo 4dδ,2,3 orbitals. The first excited state (2Π) corresponds to the 5pσ ± 5s excitation. The calculated properties of \( R_e = 1.60 \, \text{Å}, \) \( v_e = 1100 \, \text{cm}^{-1}, \) \( D_e = 4.07 \, \text{eV}, \) and \( \Delta E (2Π - 4Σ) = 2.128 \, \text{eV} \) are in good agreement with recent experimental results (\( R_e = 1.63 \, \text{Å} \) and \( \Delta E = 2.011 \, \text{eV} \)). Particularly interesting is a dramatic non-monotonic change of dipole moment with distance (\( \mu = -3.123 \, \text{D} \) at \( R = 1.60 \, \text{Å}, \) \( \mu = -0.176 \, \text{D} \) at \( R = 5.0 \, \text{Å} \)). This effect is explained.

1. Introduction

A number of systems with double and triple M–C and M–O bonds (where M is a transition metal) have now been characterized experimentally [1] and theoretically [2] and have been shown to play a role in catalytic reactions [1–3]. Although M–N double and triple bonds are believed to play a role in some catalytic processes (e.g., Mo=NR and Mo=NR in nitrogenase [4] and Mo=NR in ammoxidation catalysts [5]), few such cases have been studied experimentally or theoretically. On the experimental side, Dunn and co-workers [6] have examined the spectra of a number of transition metal nitrides, one of which is Mo=N. As part of a project to examine the role of Mo–N moieties in catalytic reactions, we have examined the ground and excited states of Mo=N and compared the results with current experimental data.

2. Character of the Mo=N bond

Mo has an s^1d^5 ground state with six electrons in separate orbitals, while N has an s^2p^3 ground

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Fig. 1. GVB orbitals for the σ bond of MoN(4Σ−) 1 as a function of internuclear distance. Note the conversion of Mo 4d,2-like orbital at 1.60 Å (\( R_e \)) to an Mo 5s-like orbital at \( R = 5.00 \, \text{Å} \). Contour increments (au) noted in the lower left-hand corner. Solid lines indicate positive contours and dashed lines negative contours; the nodal lines are not shown.
state with electrons in three separate p orbitals. Thus we expect a triple bond \((\sigma, \pi_\alpha, \pi_\beta)\) with the Mo retaining three unpaired electrons \((\delta_x, \delta_y, \delta_z, \sigma)\) leading to a \(\Sigma^-\) state. An important question is whether the Mo part of the \(\sigma\) bond involves the 5s orbital, the 4d orbital, or some hybrid combination. As indicated in fig. 1, we find indeed that at large \(R\) (5.0 Å) the \(\sigma\)-bond involves nearly pure 5s orbital but that the character changes rapidly to 4d-like at 2.5 Å and remains 4d-like at \(R_e\) (1.60 Å). At \(R_e\) the triple bond is highly covalent and involves Mo d-like orbitals in all three bonds (see figs. 1 and 2). This leaves the two \(d_\pi\) orbitals and a 5s-like orbital for three non-bonding valence electrons. This non-binding \(\sigma\) orbital is shown in fig. 3 where we see that it changes from 4d\(_{\pi}\)-like at large \(R\) to 5s-like at \(R_e\).

Because of the disparity between the sizes of the 4d\(_{\pi}\) and 5s orbitals, plots of contours with equal amplitude spacing lead to numerous contours for 4d\(_{\pi}\) but few for 5s, providing the illusion of 4d character in an orbital that is mainly 5s. In order to help display the full character of orbitals with 5s character, several of the plots in figs. 1 and 3 contain contours at 0.0250 au spacing rather than 0.050 au spacing, as indicated in the lower left portion of each figure.

In order to provide a more quantitative description of the atomic character of these orbitals, we have calculated Mulliken populations for the MoN \(\sigma\) bond and for the Mo \(\sigma\) non-bonded, singly occupied orbital of the full GVB wavefunction. These results are shown in table 1 and fig. 4. At \(R_e\), GVB calculations indicate there are 0.76 Mo d electrons in the \(\sigma\) bond, which decreases to 0.04 Mo d electrons at \(R = 5.00\) Å. As the d character decreases in the \(\sigma\) bond, the d character increases in the singly occupied Mo \(\sigma\) non-bonded Mo orbital (from 0.10 e at \(R_e = 1.6\) Å to 0.94 e at \(R = 5.0\) Å).

Fig. 2. GVB orbitals for the \(\sigma\) bond of MoN(\(4\Sigma^-\)) as a function of internuclear distance.

Fig. 3. (a) Singly occupied \(\sigma\) non-bonded orbital of MoN(\(4\Sigma^-\)) as a function of internuclear distance. Note the conversion of the diffuse Mo 5s-like orbital at \(R = 1.60\) Å \((R_e)\) to a Mo 4d\(_{\pi}\)-like orbital at \(R = 5.00\) Å. (b) Singly occupied MoN(\(\Sigma^+\)) \(\pi\) non-bonded orbital as a function of internuclear distance. Note the increasing Mo 4d\(_{\pi}\) character as \(R\) is increased.
In fig. 4 we see that at $R = 2.47 \text{ Å}$ the number of electrons in the $\sigma$ bond is equal to the number in the non-bonding orbital. In the sections 3 and 4 we will find that the total dipole moment is a maximum at this point.

From fig. 4 we see that the total number of Mo d electrons in the $\sigma$ bond plus Mo non-bonding orbital is essentially unity for $R > 3.0 \text{ Å}$ but drops to 0.80 near $R_c$.

The reason for the change in character of the $\sigma$ bond is as follows. The exchange energy for Mo($^7$S) in the s$^1$d$^5$ configuration is

$$E^{\text{ex}} = -10K_{dd} - 5K_{sd},$$

where $K_{dd} = 0.540 \text{ eV}$ and $K_{sd} = 0.306 \text{ eV}$.

If the $s$ orbital is used in a perfect valence bond to another atom, the exchange energy becomes

$$E^{\text{ex}}(s \text{ bond}) = -10K_{dd} - \frac{5}{2}K_{sd},$$

and the bond energy can be written as

$$D(s \text{ bond}) = D_s - \frac{5}{2}K_{sd} = D_s - 0.765 \text{ eV},$$

where $D_s$ is the bond strength ignoring exchange terms.

If, instead, a $d$ orbital is used in a perfect valence bond to another atom, the exchange energy becomes

$$E^{\text{ex}}(d \text{ bond}) = -8K_{dd} - \frac{3}{2}K_{sd},$$

and the bond energy will be written as

$$D(d \text{ bond}) = D_d - 2K_{dd} - \frac{3}{2}K_{sd} = D_d - 1.233 \text{ eV}.$$
bond is favored. This trend is aided by the two \( \pi \) bonds. Thus the exchange interaction for one \( \sigma \) bond and two \( 4d\pi \) bonds is

\[
E^-\pi(\sigma, \pi, \pi) = -\frac{1}{3} K_{4d} - \frac{2}{3} K_{d\pi},
\]

while for one \( d\sigma \) bond and two \( 4d\pi \) bonds it is

\[
E^-\pi(d\sigma, \pi, \pi) = -\frac{1}{3} K_{dd} - \frac{2}{3} K_{d\pi}
\]

leading to

\[
D(\sigma, d\pi, d\pi) = D_{\sigma} + 2D_{d\pi} - \frac{2}{3} K_{dd} - \frac{1}{3} K_{d\pi}
\]

\[
D(d\sigma, d\pi, d\pi) = D_{d\sigma} + 2D_{d\pi} - \frac{2}{3} K_{dd} - \frac{1}{3} K_{d\pi}
\]

Thus, because of the \( \pi \) bonds, the loss in exchange stabilization due to a \( d\sigma \) bond is reduced, leading to increased \( d \) character in the bond. These factors explain the overall character of fig. 4.

### 3. Dipole moment of MoN\((4\Sigma^-)\)

In fig. 5 we show the dipole moment (solid line) for \( 4\Sigma^- \) MoN. At \( R_e \) the dipole moment is large (\(-3.123 \text{ debye} = -1.229 \text{ au}\)) and negative (corresponding to Mo\(^+\)N\(^-\)). In a point-charge model this dipole moment would correspond to a charge transfer of 0.41 electrons from Mo to N. Note-worthy here is that the dipole moment does not change monotonically with \( R \). Thus the dipole moment is a maximum (\(-5.982 \text{ debye} = -2.353 \text{ au}\)) at \( R = 2.60 \text{ Å} \), a distance 62% larger than \( R_e \).

In order to examine the origin of this behavior, we have partitioned the total dipole into three parts: the contribution from the Mo non-bonded orbitals plus core orbitals; the contribution from the MoN \( \sigma \) bond; and finally, the contribution from the two \( \pi \) bonds. These results are listed in table 2 and plotted in fig. 5. At \( R = 5.0 \text{ Å} \) the various components of the dipole moment are all small. As \( R \) is decreased from 5.0 \( \text{ Å} \), the \( s \) character in the \( \sigma \) bond decreases and the \( d \) character increases so that by \( R = 2.50 \text{ Å} \) an equal amount of \( s \) and \( d \) character is present (see fig. 4). This is the region in which the magnitude of the total MoN dipole moment is the greatest, \(-2.353 \text{ au}\) (see fig. 5), with the polarity Mo\(^+\)N\(^-\). As \( R \) is decreased further, the magnitude of the dipole moment decreases to \(-3.123 \text{ debye} (\sim 1.2288 \text{ au})\) at \( R_e = 1.60 \text{ Å} \), still with the polarity Mo\(^+\)N\(^-\).

When the bond has Mo \( s \) character, there are two factors favoring a dipole moment with sign Mo\(^+\)N\(^-\). First, the 5s orbital is easily polarized using the empty 5p orbital to obtain greater overlap with the N, whereas the 4d orbital is more costly to polarize (requiring a 4f-like orbital for maximal polarization). Secondly, the 5s IP (7.10 eV) [8] is much less than the 4d IP (8.56 eV) [8], allowing greater charge transfer. For example, at \( R = 2 \text{ Å} \), the strength of a purely-ionic bond (ignoring overlap effects) would be

\[
D_{s\text{ion}}(\text{eV}) = EA(N) + 14.4/R(A) - IP(Mo\ 5s) = 0.10 \text{ eV}.
\]

\[
D_{d\text{ion}}(\text{eV}) = EA(N) + 14.4/R(A) - IP(Mo\ 4d) = -1.36 \text{ eV}.
\]

for \( s \) and \( d \) bonds, respectively. This indicates that charge transfer will be important if the bond has Mo \( s \) character but not if it has Mo \( d \) character.

As \( R \) decreases from \( \infty \) to 2.6 \( \text{ Å} \), the charge transfer in the bond increases due to the greater favoring of ionic character (the \( 1/R \) term) despite the gradual increase in \( d \) character. As the bond becomes dominated by the \( d \) character for smaller
there can be little charge transfer, leading to a dipole moment contribution at small $R$ that is small ($-0.64 \text{ D}$). The result then is a Morse-like dipole contribution from the $\sigma$ bond, with a minimum of $-5.98 \text{ D}$ at $2.67 \text{ Å}$.

In addition to the above contributions from the $\sigma$ bond, we find that for $R < 1.8 \text{ Å}$ the $\pi$ system dominates. This is due to the charge transfer associated with the MoN covalent $\pi$ bonds at smaller $R$. Note that for $R > 2.6 \text{ Å}$ the $\pi$ system responds to the Mo$^+$ N$^-$ character in the $\sigma$ system by donation of N$\pi$ character to the molybdenum (fig. 5).

4. Dipole moment of MoN($^4\Pi$)

Similar non-monotonic behavior regarding the trend of the total dipole moment is also found for the $^4\Pi$ excited state (fig. 6). Just as there is a choice for MoN($^4\Sigma^-$) between bonding an Mo 5s or Mo 4d$_{xz}$ orbital to the N 2p$_x$ orbital, there is an analogous situation for the $\pi$ system for MoN($^4\Pi$). As Mo($^7\text{P}$) and N($^4\text{S}$) are brought together from their atomic limits, there is a choice between bonding an Mo 5p$_x$ or Mo 4d$_{xz}$ orbital to the N 2p$_x$ orbital.

At large distances, the exchange terms favor bonding of the Mo 5p$_x$ over Mo 4d$_{xz}$ and the IP (IP$_{5p} = 3.89 \text{ eV}$ versus IP$_{4d} = 9.74 \text{ eV}$) [8] is such that the charge transfer is even larger than for MoN($^4\Sigma^-$). At smaller $R$, the larger covalent bond strength possible for Mo 4d$_{xz}$ leads to increased d character and eventually a decrease in the charge transfer. This results in a maximum in the dipole moment of $\mu(3.25 \text{ Å}) = -4.542 \text{ au} = -11.545 \text{ D}$ (see fig. 7) with polarity Mo$^+$ N$^-$ (corresponding to a transfer of 0.75 electrons from Mo to N). As $R$ is decreased from $3.0 \text{ Å}$ to $R_e = 1.59 \text{ Å}$, the magnitude of the dipole decreases to $-1.793 \text{ au} = -4.556 \text{ D}$, still with polarity Mo$^+$ N$^-$. As $R$ is decreased further and approaches $2.0 \text{ Å}$, the $\pi$ bonding becomes more covalent, involving primarily to Mo 4d$_{xz}$ and N 2p$_x$ orbitals. The overall

![Fig. 6. GVB orbitals for the $\pi$ bond of MoN($^4\Pi$) as a function of internuclear distance.](image-url)
effect is shown by a change in sign of the dipole derivative at $R = 3.25$ Å, which is where the N 2p$_z$ orbital begins to donate charge back to the Mo 4d$_{xz}$ orbital.

5. Spectroscopic properties and the excited state

The first excited state of MoN corresponds to excitation of the 5s-like non-bonding orbital into a 5p $\pi$-like orbital, leading to a $^3\Pi$ state. The potential energy curves of these states are shown in fig. 8 and the spectroscopic properties tabulated in table 3. We find (see table 3) that removal of the non-bonding $\sigma$ electron leads to a slightly longer $R_e$ (by 0.005 Å) and a smaller vibrational frequency (by 200 cm$^{-1}$). The total excitation energy is calculated to be 2.13 eV = 17 166 cm$^{-1}$, which is in good agreement with the experimental value of 2.01 eV = 16 217 cm$^{-1}$ [6].

6. Calculational details

Electron correlation is extremely important for a system such as Mo=N with multiple bonds. Thus, the Hartree–Fock (HF) description gives a bond distance too short by $\approx 0.1$ Å and shows MoN to be unbound by 0.35 eV (see fig. 9).

Wavefunctions. In order to adequately describe the bonding in MoN, we have carried out calculations using generalized valence bond (GVB) and GVB RCI wavefunctions in which the three pairs

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**Table 3**

Spectroscopic properties for MoN from the full GVB calculation (GVB-3)

<table>
<thead>
<tr>
<th>State</th>
<th>Total energy (hartree)</th>
<th>Bond dissociation energy $D_e$ (eV)</th>
<th>Bond distance (Å)</th>
<th>Force constant $k$ (hartree/Å$^2$)</th>
<th>Harmonic vibrational frequency $\omega_e$ (cm$^{-1}$)</th>
<th>Excitation energy $E_e$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^4\Sigma$</td>
<td>-102.773612</td>
<td>4.075$^{a4}$</td>
<td>1.603</td>
<td>1.633</td>
<td>2.0076</td>
<td>1100.4</td>
</tr>
<tr>
<td>$^4\Pi$</td>
<td>102.695397</td>
<td>4.639$^{b4}$</td>
<td>1.608</td>
<td>1.654</td>
<td>1.3419</td>
<td>899.6</td>
</tr>
</tbody>
</table>

$^{a4}$ For MoN($^4\Sigma$), the $D_e$ is with respect to ($^5\Sigma$) Mo and ($^4\Sigma$) N atomic limits.

$^{b4}$ For MoN($^4\Pi$), the $D_e$ is with respect to ($^3\Pi$) Mo and ($^4\Sigma$) N atomic limits.

$^{c4}$ Calculated from rotational constant $B_0$ in ref. [6].

$^{d4}$ See ref. [6].

$^{e4}$ Calculations on the atoms yield $E(Mo) = -48.239487$ hartree and $E(N) = -54.394390$ hartree.

$^{f4}$ To convert to dynes/cm, multiply by $4.359814 \times 10^5$. 

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![Dipole moment](image1.png)

**Fig. 7** Total dipole moment of MoN($^4\Pi$) as a function of internuclear distance.

![Potential curves](image2.png)

**Fig. 8** Potential curves for the ($^4\Sigma$) ground state and ($^4\Pi$) excited state of MoN using the full GVB wavefunction. The energy (eV) is relative to Mo ($^5\Sigma$) and N ($^4\Sigma$) HF atomic limits.
of bonding orbitals (one σ and two π) have been correlated. In fig. 9 we show the results of a GVB perfect pairing (GVB PP) calculation leading to a bond dissociation energy $D_e$ of 1.93 eV with respect to the appropriate atomic limits. Using the perfect-pairing restriction, the GVB wavefunction (denoted GVB PP) dissociates properly to the atomic fragments but not to the proper spin state [Mo($^7S$) and N($^4S$)]. The reason is that the three bond pairs remain singlet-coupled, prohibiting the high-spin coupling of the orbitals on each atom as dissociation occurs.

A common way to solve this problem is to use the orbitals from the GVB PP wavefunction but to allow them to be combined so as to describe a general spin-coupling of the electrons. This is accomplished by a small configuration interaction (CI) calculation (referred to as GVB RCI) in which the two electrons of each singlet pair from GVB PP are allowed any occupation of the two orbitals of that pair. In a CI description, the GVB PP wavefunction of MoN($^4Σ^-$) would have $2^3 = 8$ configurations, each with three open-shell (unpaired) electrons. In the GVB RCI description, there are $3^3 = 27$ spatial configurations, some of which have up to nine open-shell (unpaired) electrons. The GVB RCI leads to a bond energy of 4.03 eV, a significant improvement over the value of 1.93 eV for GVB PP. (It is important to allow a total of nine open shells (three singly occupied Mo orbitals plus six GVB orbitals involving three bond pairs); thus, if only five open shells are allowed, the calculated $D_e$ is only 2.20 eV.)

Although the GVB RCI gives a quantitatively good description for small $R$, it dissociates to a limit just slightly above that of the high-spin products. This is because the orbitals (obtained from GVB PP) have incorrect shapes. The result is a small hump in the potential curve (0.36 eV at 3.00 Å). In order to obtain the optimum orbitals while including the optimum spin coupling, we use the GVB3 program [9] in which all orbitals are solved for self-consistently for the full 27 configurations of the RCI wavefunction (188 spin eigenfunctions). This corresponds closely to the full GVB wavefunction including spin-coupling optimization. As indicated in fig. 9, the GVB wavefunction dissociates monotonically to the Mo($^7S$) and N($^4S$) limit. At $R_e$ the full GVB wavefunction leads to a bond energy of 4.07 eV, just slightly better than GVB RCI (4.071 eV). Total energies, the equilibrium internuclear distance, and bond dissociation energies for the various wavefunctions are shown in table 4.

As a final wavefunction, we allowed all single excitations from all occupied orbitals of the 27 GVB RCI configurations to all the virtual orbitals (1199 configurations and 10 592 spin eigenfunctions). This is referred to as GVB•S (for full GVB

<table>
<thead>
<tr>
<th>Table 4</th>
<th>Total energies (hartree) for MoN($^4Σ^-$) at selected distances</th>
</tr>
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<tr>
<td>$R = 1.60 Å$</td>
<td>$R = 5.00 Å$</td>
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<tr>
<td>HF</td>
<td>-102.604386</td>
</tr>
<tr>
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<td>GVB RCI</td>
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<tr>
<td>GVB</td>
<td>-102.773604</td>
</tr>
<tr>
<td>GVB•S</td>
<td>-102.791694</td>
</tr>
</tbody>
</table>
times singles). The result is a bond energy of 4.57 eV.

The spectroscopic properties in table 3 were obtained from the full GVB wavefunction, while dipole moments (table 2 and fig. 5) and orbital plots were derived from GVB PP wavefunctions. Results from table 1 and fig. 4 were obtained from the full GVB wavefunction.

The total energies of MoN($^4\Sigma^-$) and MoN($^4\Pi$) for the full GVB wavefunction at various inter-nuclear distances are tabulated in table 5.

### Table 5
Total energies (au) for MoN($^4\Sigma^-$) and MoN($^4\Pi$) as a function of internuclear distance $R(\AA)$ for the full GVB wavefunction

<table>
<thead>
<tr>
<th>$R(\AA)$</th>
<th>Energy (au)</th>
<th>MoN($^4\Sigma^-$)</th>
<th>MoN($^4\Pi$)</th>
</tr>
</thead>
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<tr>
<td>1.30</td>
<td>-102.608924</td>
<td>-102.535795</td>
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<td>1.50</td>
<td>-102.760771</td>
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<td>-102.770538</td>
<td>-102.692835</td>
<td></td>
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<td>1.60</td>
<td>-102.773604</td>
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<td>3.00</td>
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<td>5.00</td>
<td>-102.623951</td>
<td>-102.525112</td>
<td></td>
</tr>
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7. Basis set and potential

We have replaced the Zn ($Z = 30$) core of Mo ($Z = 42$) by a relativistic effective potential (Hay [10]) thereby treating Mo as a (4p)$^6$(4d)$^2$(2s)$^1$ 12-electron system. The Mo basis consisted of a [3s,4p,2d] contraction basis of a (3s,5p,3d) set of primitive gaussians and is listed in table 6. For

### Table 6
Molybdenum basis (Hay [10]). The [3s, 4p, 2d] contracted basis for Mo, $E = -48.229487$ hartree

<table>
<thead>
<tr>
<th>s basis</th>
<th>p basis</th>
<th>d basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_s$</td>
<td>$\alpha_p$</td>
<td>$\alpha_d$</td>
</tr>
<tr>
<td>$c_s$</td>
<td>$c_p$</td>
<td>$c_d$</td>
</tr>
<tr>
<td>0.6748</td>
<td>1.0000</td>
<td>9.6460</td>
</tr>
<tr>
<td>0.07682</td>
<td>1.0000</td>
<td>1.2340</td>
</tr>
<tr>
<td>0.02911</td>
<td>1.0000</td>
<td>0.4261</td>
</tr>
<tr>
<td>0.08874</td>
<td>1.0000</td>
<td>0.02660</td>
</tr>
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</table>
nitrogen, the Dunning [3s,2p] contraction of the Huzinaga (9s,5p) basis was used. We supplemented the nitrogen basis with polarization functions \((\alpha = 0.760)\) [11].

Acknowledgement

We would like to thank Dr. P. J. Hay for the use of the molybdenum effective potential. The parameters of the potential are tabulated in Table 7. We thank Professor Tom Dunn of Michigan State University for providing the experimental data and references in advance of publication [6]. Acknowledgement is made to the Donors of the Petroleum Research Fund, administered by the American Chemical Society, for the partial support of this research (Grant No. 13110-AC5,6).

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