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Photoinduced dehydrogenation of 1,4-cyclohexadiene by NO_2 in a cryogenic Ar matrix

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Abstract

Visible-light-induced dehydrogenation of 1,4-cyclohexadiene (1,4-CHD) using NO_2 was observed in a cryogenic Ar matrix. This photoinduced dehydrogenation was interpreted by the following reaction sequence (1)–(3): (1) photoexcitation of NO_2; (2) hydrogen atom transfer to form a complex of cyclohexadienyl radical and nitrous acid; (3) photodissociation of the complex into benzene + NO + water or benzene + HNO + OH. The photochemistry of 1,4-CHD–NO_2 contrasts with that observed in other unsaturated hydrocarbon–NO_2 systems, where oxygen atom transfer to form oxirane biradical and NO is the dominant reaction process. © 1997 Elsevier Science S.A.

Keywords: Cryogenic Ar matrix; 1,4-Cyclohexadiene; NO_2; Photoinduced dehydrogenation

1. Introduction

Visible-light-induced oxygen atom transfers from NO_2 to unsaturated hydrocarbons and amines have been investigated in cryogenic matrices [1–19]. These bimolecular reactions are initiated by visible light at wavelengths much longer than 398 nm, corresponding to the NO_2 dissociation threshold. In an unsaturated hydrocarbon–NO_2 system, epoxide and aldehyde are produced via transient formation of the oxirane biradical or nitrite radical. In an amine–NO_2 system, imine is produced via amine *N*-oxide formation followed by dehydration. These reactions proceed on the singlet surfaces of the oxirane biradical and amine *N*-oxide which are located below the triplet surfaces.

In this paper, we describe a new type of visible-light-induced reaction observed in a 1,4-cyclohexadiene (1,4-CHD)–NO_2 system. Hydrogen atom transfer is dominant over oxygen atom transfer. The weakness of the C–H bond in 1,4-CHD seems to play an important role. The nitrous acid produced is found to be weakly perturbed by the coproduct, cyclohexadienyl radical.

2. Experimental details

The experimental set-up is similar to that described previously [16]. Briefly, light irradiation was performed using an Ar^+ laser (Spectra Physics, Stabilite 2016) or an Ar^+-laser-pumped dye laser (Spectra Physics, Model 375 B). The Ar^+ laser was operated in all- or single-line mode. Rhodamine 6G was used as laser dye.

IR spectra were measured in the range 4600–600 cm^{-1} with 0.5 cm^{-1} resolution by a JASCO 8000S Fourier transform IR spectrometer with a liquid-nitrogen-cooled MCT detector. Each spectrum was obtained by scanning over 100 times. A closed-cycle helium cryostat (Cryogenic Technology Inc., Model 21 Cryodyne) was used to control the temperature of the Ar matrix.

Argon gas (Takachiho, 99.9999% purity) was used without further purification. NO_2 (Sumitomo Seika, pure grade) was purified by freeze–pump–thaw cycling at 77 and 193 K. An isotopic NO_2 mixture was prepared by oxidation of $N^{16}O$ (Takachiho) by $^{18}O_2$ (Matheson, 99 at.% ^{18}O). The $N^{16}O_2/N^{16}O^{18}O/N^{18}O_2$ isotope ratio was 0.44:0.44:0.13 or 0.15:0.30:0.55. 1,4-CHD (Aldrich, 97%) and benzene (Wako Pure Chemical) were used after freeze–pump–thaw cycling at 77 K. 1,4-CHD and NO_2 were diluted independently with argon. Samples were codeposited on a CsI window at 16 K.

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3. Results

Mixtures of 1,4-CHD–Ar and NO_2–Ar were codeposited on a CsI window with a 1,4-CHD/NO_2/Ar ratio of 5:1:100 or 2.5:1:200. In the IR spectrum obtained after codeposition, strong bands due to NO_2 and 1,4-CHD were observed [20,21]. The spectrum also contained additional weak bands due to N_2O_4 and N_2O_3. Irradiation with light longer than 630 nm did not cause the reaction of NO_2 with 1,4-CHD, but N_2O_3 isomerization occurred [20]. Irradiation at wavelengths shorter than 615 nm resulted in the appearance of new bands, which were not assigned to N_xO_y, with a decrease in the intensities of the bands due to the reactants 1,4-CHD and NO_2. Fig. 1 shows the IR difference spectrum obtained on 574 nm irradiation of a 1,4-CHD–NO_2–Ar matrix. The positive and negative bands indicate the growth and depletion respectively during the irradiation period. Table 1 displays the frequencies of the product bands generated by the photochemical reaction of NO_2 with 1,4-CHD. Of the product absorptions, the bands at 3443, 3300, 1672, 1620, 867, 819 and 632 cm^{-1} increased with constant relative intensities during the irradiation period, and were attributed to a single molecule, species A. The baseline in the 3500–3100 cm^{-1} region was not flat due to interference caused by amorphous water accumulated on the matrix surface. In addition, two strong bands were observed at 1647 and 757 cm^{-1} (species B). The relative intensities of the bands due to species A and B were dependent on the light wavelength used. At shorter wavelengths, predominantly species A was produced. For the reaction using an isotopic NO_2 mixture, the bands due to species A shifted from 3443, 3300, 1672, 867 and 819 cm^{-1} to 3420, 3285, 1638, approximately 850 (858, 850 and 845) and approximately 810 cm^{-1} respectively. Fig. 2 shows the isotope shifts of species A in the 900–780 cm^{-1} region. Spectra (a), (b) and (c) were measured using NO_2 with different $N^{16}O_2/N^{18}O^{16}O/N^{18}O_2$ isotope ratios. The weak bands at 1482, 1037 and 682 cm^{-1} in the experiments using normal $N^{16}O_2$ did not shift in the experiments using isotopic NO_2. A product band at 1872 cm^{-1}, whose isotopic counterpart appeared at 1823 cm^{-1}, was due to NO [2]. The bands at 2754 and 1560 cm^{-1} were assigned to the NH and NO

Table 1
IR spectra obtained on visible light irradiation of the matrix 1,4-CHD–NO_2–Ar

ν (cm^{-1})	Irradiation (nm) [a]		Species
	574	457.9–514.5	
3545	+	+	OH
3443	+	−	A [b]
3300	+	−	A
3096		+	Benzene
2754	+	+	HNO
1872	+	+	NO
1672	+	−	A
1647	+	−	B [c]
1620	+	−	A
1560	+	+	HNO
1482	+	+	Benzene
1426	+	−	C [d]
1037	+	+	Benzene
1015	+	−	C
910	+	−	B
867	+	−	A
819	+	−	A
757	+	−	B
682	+	+	Benzene
632	+	−	A

[a] Signs of + and − indicate the positive and negative changes respectively in the difference spectra on laser irradiation.
[b] A denotes nitrous acid.
[c] B denotes cyclohexenyl nitrite radical.
[d] C denotes cyclohexadienyl radical.

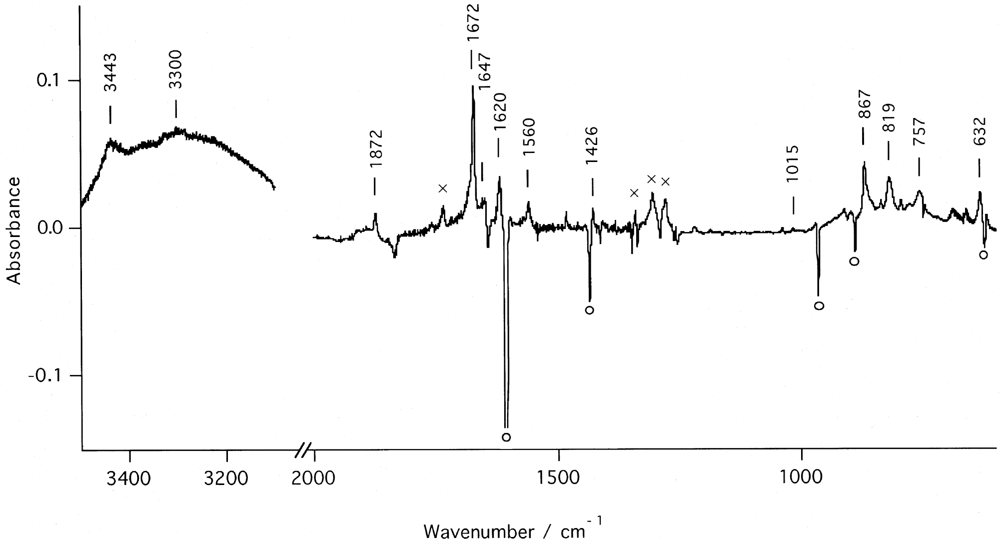

Fig. 1. IR difference spectrum on 574 nm (400 mW cm^{-2}) irradiation of the matrix 1,4-CHD–NO_2–Ar (5:1:100) for 7 h. The decreased bands due to the reactants (1,4-CHD and NO_2) are indicated by ○. The absorption changes due to N_2O_4 production (dimerization of NO_2) and $CsNO_x$ production are indicated by ×.

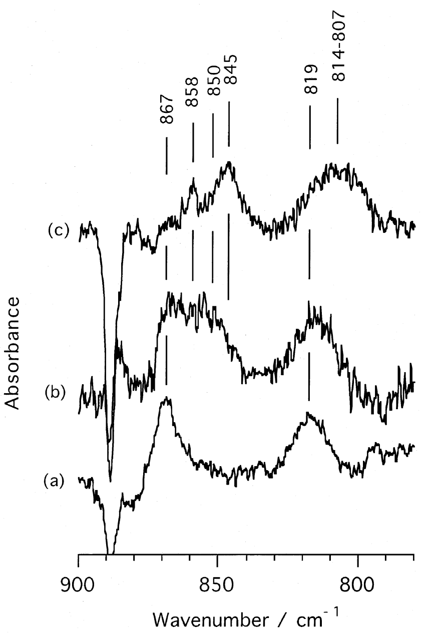

Fig. 2. IR difference spectra at 900–780 cm^{-1} on 574 nm irradiation of the matrix 1,4-CHD–NO$_2$–Ar with N^{16}O$_2$/N^{18}O^{16}O/N^{18}O$_2$ isotope ratios: (a) 1:0:0; (b) 0.44:0.44:0.13; (c) 0.15:0.30:0.55.

stretching fundamentals of HNO respectively by comparison with the spectrum measured in an argon matrix [22]. The band at 3545 cm^{-1} was assigned to OH [23].

Fig. 3 shows the spectral changes observed on further irradiation of the matrix containing species A with 457.9–514.5 nm light (all-line operation) at 100 mW cm^{-2} for 1 min. The spectral changes are summarized in the third column of Table 1. The bands due to species A showed a decrease in intensity, while the bands at 1482, 1037 and 682 cm^{-1} and that due to NO showed a further increase.

When a 1,4-CHD–NO$_2$–Ar matrix was irradiated with 514.5 nm light (single-line operation, 200 mW cm^{-2}), the bands due to species A reached a maximum intensity around 30 min and then started to decrease on continued irradiation. The NO band and the bands at 3096, 1482, 1037 and 682 cm^{-1} continued to increase for at least 3 h. We assigned the last four bands to a single molecule, benzene, by comparison with a matrix isolation spectrum of authentic benzene [24].

4. Discussion

4.1. Identification of products

Species A and B exhibit strong bands in the IR regions characteristic of N=O and N–O stretches observed for alkyl nitrite radicals. However, alkyl nitrite radicals do not have a 3443 cm^{-1} band belonging to species A. The frequencies of species A (3443, 3300, 1672, 1620, 867, 819 and 632 cm^{-1}) are close to those of *trans*- and *cis*-nitrous acid (3573, 3412, 1689, 1634, 853, 800 and 638 cm^{-1} [25]). Therefore we assign species A to *trans*- and *cis*-HONO. The fundamental frequencies of *trans*- and *cis*-HONO are listed in Table 2 and Table 3 respectively. The assignment of the observed bands to the trans and cis isomers is based on the characteristic IR frequencies of the two isomers measured in argon matrices [25]. The broad 3443 and 3300 cm^{-1} bands appearing in the O–H stretching region shift to 3420 and 3285 cm^{-1} respectively when isotopic NO$_2$ is used. These isotope shifts agree with the observation for the O–H fundamental of HONO [26,27]. The 1672 and 1620 cm^{-1} bands observed in the N=O stretching region are assigned to the N=O stretching of *trans*- and *cis*-HONO respectively. The 1672 cm^{-1} band shows an ^{18}O isotope shift of 34 cm^{-1}. The isotopic counterpart band for 1620 cm^{-1} is not observed, possibly due to overlap with a strong N^{18}O^{16}O depletion band. Overlap is expected if the value of the isotope shift is the same as the 1672 and 1620 cm^{-1} bands. The bands at 867 and 819 cm^{-1} are assigned to the N–O stretching of *cis*- and *trans*-HONO

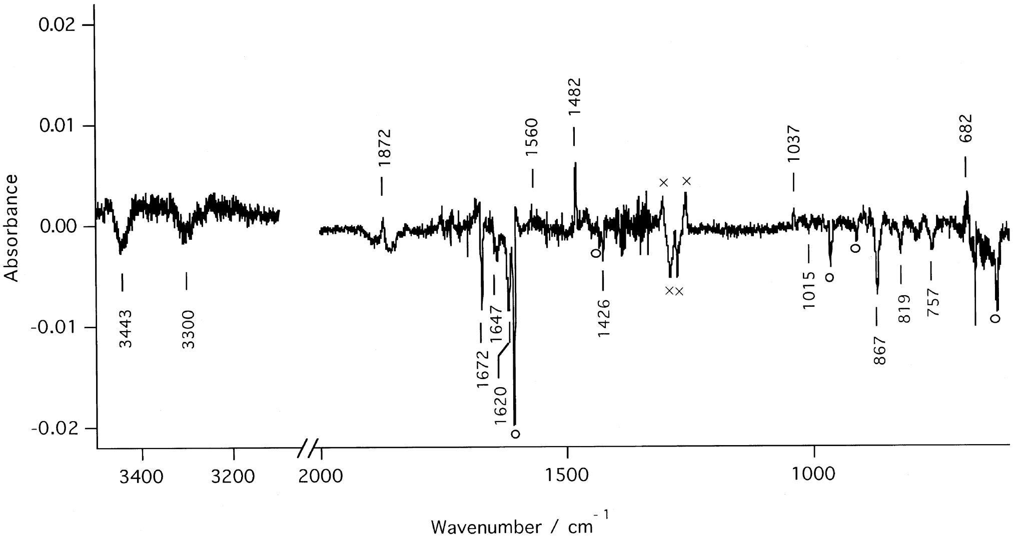

Fig. 3. IR difference spectrum on 1 min irradiation at 457.9–514.5 nm (Ar$^+$ laser, 100 mW cm^{-2}) of the 1,4-CHD–NO$_2$–Ar matrix subsequent to 7 h irradiation at 574 nm (500 mW cm^{-2}) as explained for Fig. 1. The decreased bands due to 1,4-CHD and NO$_2$ are indicated by ○. The absorption changes due to N$_x$O$_y$ are indicated by ×.

Table 2
IR absorptions and assignments of *trans*-HONO in an Ar matrix

ν (cm^{-1})				Assignment
$C_6H_7\cdots HONO$	$H_3N\cdots HONO$ [a]	HONO [b]	HONO [c]	
3443	2765.2	3551		O–H stretch, $H^{16}ON^{16}O/H^{16}ON^{18}O$
3420		3536		O–H stretch, $H^{18}ON^{18}O/H^{18}ON^{16}O$
1672		1682	1690	N=O stretch, $H^{16}ON^{16}O/H^{18}ON^{16}O$
1638		1641		N=O stretch, $H^{18}ON^{18}O/H^{16}ON^{18}O$
819	883.5	814	800	N–O stretch, $H^{16}ON^{16}O$
814–807		810, 804	800–787	N–O stretch, isotopic HONO

[a] In an Ar matrix [25].
[b] In an N_2 matrix [26].
[c] In an Ar matrix [27].

Table 3
IR absorptions and assignments of *cis*-HONO in an Ar matrix

ν (cm^{-1})				Assignment
$C_6H_7\cdots HONO$	$H_3N\cdots HONO$ [a]	HONO [b]	HONO [c]	
3300		3410	3412	O–H stretch, $H^{16}ON^{16}O/H^{16}ON^{18}O$
3285		3404	3402	O–H stretch, $H^{18}ON^{18}O/H^{18}ON^{16}O$
1620		1629	1633	N=O stretch, $H^{16}ON^{16}O/H^{18}ON^{16}O$
n.d. [d]		1589		N=O stretch, $H^{18}ON^{18}O/H^{16}ON^{18}O$
867	947.5	864	850	N–O stretch, $H^{16}ON^{16}O$
858		859	846	N–O stretch, $H^{16}ON^{18}O$
850		850	836	N–O stretch, $H^{18}ON^{16}O$
845			836	N–O stretch, $H^{18}ON^{18}O$
632		662	637	O–H torsion, $H^{16}ON^{16}O$
n.d. [d]			635	O–H torsion, isotopic HONO

[a] In an Ar matrix [25].
[b] In an N_2 matrix [26].
[c] In an Ar matrix [27].
[d] Not determined, see text.

respectively. They are blue shifted by 17 and 19 cm^{-1} respectively from the corresponding monomer band of HONO. In the isotopic experiments, the 867 cm^{-1} band is red shifted and split into four bands (867, 858, 850 and 845 cm^{-1}) corresponding to the four isotope-labelled *cis*-HONO species ($H^{16}ON^{16}O$, $H^{16}ON^{18}O$, $H^{18}ON^{16}O$ and $H^{18}ON^{18}O$ respectively). The 819 cm^{-1} band is isotope shifted to a broad band, the centre position of which changes from 819 to 807 cm^{-1} depending on the isotope ratios as shown in Fig. 2. Possibly, four bands are overlapped with each other [26,27]. The 632 cm^{-1} band is assigned to the OH torsion of *cis*-HONO. Unfortunately, the 632 cm^{-1} band is close to a strong depletion band of 1,4-CHD. Therefore the frequency will be the upper limit and the isotope-shifted band cannot be recognized in the present experiment.

On 574 nm irradiation of NO_2–1,4-CHD, we observe the formation of *cis*- and *trans*-HONO, whose vibrational frequencies are deviated from those measured under isolated conditions. Subsequent irradiation at 457.9–514.5 nm results in the formation of benzene. These observations suggest that HONO and the coproduct, cyclohexadienyl radical, exist as intermediates in a matrix cage. The candidate bands for the coproduct are those at 1426 and 1015 cm^{-1} (species C), whose photochemical behaviour is similar to that of HONO. The frequencies of 1426 and 1015 cm^{-1} are close to the 1439 and 962 cm^{-1} bands of 1,4-CHD associated with the C=C stretching vibration. The absorption bands of C_6H_5D and C_6H_6F, where the D_{6h} symmetry of benzene is distorted and lowered, have been reported to appear around 1450 and 1000 cm^{-1} [28]. Thus species C is tentatively assigned to the cyclohexadienyl radical.

Judging from the fact that the IR absorption bands due to HONO are shifted from the isolated bands, and the directions of the shifts are in agreement with those observed in an $H_3N\cdots HONO$ complex, HONO probably forms a weakly bonded complex with the coproduct, cyclohexadienyl radical.

The 1647 and 757 cm^{-1} bands of species B are assigned to the N=O and N–O stretching vibrations respectively of the cyclohexenyl nitrite radical. The structure of 1,4-CHD has been reported theoretically [29,30] and experimentally [31] to be planar. The oxirane biradical formed may exist in two stable half-chair conformations similar to cyclohexene [29], namely one with an axial C–O bond and the other with an equatorial C–O bond. The nitrite radical formed by NO

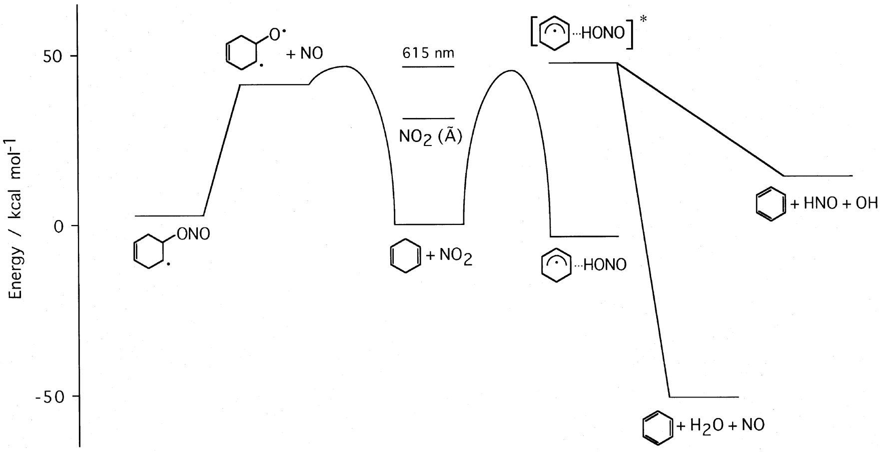

Fig. 4. Energy diagram for the photoreaction of NO_2 with 1,4-CHD.

recombination with the oxirane biradical may show these two conformations. However, only one pair of N=O and N–O stretching vibrations is observed. Therefore one of the conformers is produced predominantly. By comparison with the observed frequencies of the cyclohexyl nitrite radical [5], the nitrite radical produced by the photochemical reaction of NO_2 with 1,4-CHD has an equatorial C–O bond.

The bandwidth of the 682 cm^{-1} band, which corresponds to the out-of-plane C–H bending fundamental of benzene [24], is broader than those of the 1482 and 1037 cm^{-1} bands, corresponding to the in-plane C–H bending and C–C deforming fundamentals respectively. This observation suggests that benzene is mainly perturbed by the coproduct(s) from the flat side of the benzene ring, e.g. a benzene··· water complex [32,33].

4.2. Reaction mechanism

Fig. 4 shows the energetics of the reaction initiated by 457.9–615 nm irradiation of 1,4-CHD–NO_2. These energetics are derived from the heats of formation [34,35]. We neglect the binding energy caused by complexation.

The initial step involves hydrogen atom abstraction of 1,4-CHD by NO_2 caused by visible light irradiation to form nitrous acid and the cyclohexadienyl radical. The two photochemical products form a complex and the IR absorptions of HONO are deviated from those of the isolated molecule. In the present system, oxygen atom transfer is a minor process, which contrasts with the results obtained in other unsaturated hydrocarbon–NO_2 systems.

1,4-CHD absorbs UV light to decompose into H_2 and benzene [36]. However, direct dehydrogenation can be ruled out for energetic reasons. Therefore it is reasonable to consider that benzene is obtained by the sequential photochemical reaction of the complex or by unimolecular dissociation of the excited complex. The low energy photodissociation processes of HONO are reported as follows [37]

$$\mathrm{HONO} + h\nu \rightarrow \mathrm{HO} + \mathrm{NO} \quad \Delta H^\circ = 48.3\ \mathrm{kcal\ mol^{-1}} \tag{1}$$

$$\mathrm{HONO} + h\nu \rightarrow \mathrm{H} + \mathrm{NO_2} \quad \Delta H^\circ = 77.9\ \mathrm{kcal\ mol^{-1}} \tag{2}$$

The threshold wavelengths for reactions (1) and (2) are 591 and 367 nm respectively. The weak photoabsorption of HONO is reported to take place below 585 nm [38]. Under the present experimental conditions, only process (1) can take place. On 574 nm irradiation, HNO and benzene are formed. Thus we consider that the hydrogen atom of the cyclohexadienyl radical is abstracted by NO or OH produced by HONO photodissociation. The bond energy of the methylene C–H bond of the cyclohexadienyl radical is only 24 kcal mol^{-1} [34] and this bond may be easily cleaved.

On 457.9–514.5 nm irradiation, another process for the production of benzene is possible. The cyclohexadienyl radical exhibits an electronic transition at 559 nm [39]. Photodissociation of the cyclohexadienyl radical occurs to yield benzene and a hydrogen atom. The hydrogen atom can react further with adjacent HONO to produce $NO + H_2O$ or HNO + OH. Unfortunately, the 3750–3600 cm^{-1} region of the spectrum is perturbed by atmospheric water absorption. We cannot distinguish between the water absorption isolated or complexed with benzene in the matrix [32]. Different photochemical behaviour of complexed *cis*- and *trans*-HONO is observed on light irradiation at 574 and 457.9–514.9 nm, which is recognized by comparing the relative intensities of the 1672 and 1620 cm^{-1} bands of Fig. 1 and Fig. 3. The main photoreaction scheme of 1,4-CHD–NO_2 is summarized as follows

$$\mathrm{NO_2} + h\nu \rightarrow \mathrm{NO_2^*} \tag{3}$$

$$\mathrm{C_6H_8} + \mathrm{NO_2^*} \rightarrow \mathrm{C_6H_7} \cdots \mathrm{HONO} \tag{4}$$

$$\mathrm{C_6H_7} \cdots \mathrm{HONO} + h\nu \rightarrow \mathrm{C_6H_6} + \mathrm{NO} + \mathrm{H_2O} \tag{5}$$

$$\mathrm{C_6H_7} \cdots \mathrm{HONO} + h\nu \rightarrow \mathrm{C_6H_6} + \mathrm{HNO} + \mathrm{OH} \tag{6}$$

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