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DEPARTMENT OF DEFENSE
UNITED STATES OF AMERICA

Defense Nuclear Agency
Alexandria, VA 22310-3398

DNA-TR-90-94

Kinetic Branching of the $N^* + O_2$ Reaction

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December 1990

Technical Report

CONTRACT No. DNA 001-88-C-0032

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REPORT DOCUMENTATION PAGE

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1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
901201

3. REPORT TYPE AND DATES COVERED
Technical — 890415 - 900415

4. TITLE AND SUBTITLE
Kinetic Branching of the $N^* + O_2$ Reaction

5. FUNDING NUMBERS
C - DNA 001-88-C-0032
PE - 63220C
PR - SA
TA - SA
WU - DH048180

6. AUTHOR(S)
H. H. Michels

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
United Technologies Corporation
Research Center
Silver Lane
East Hartford, CT 06108

8. PERFORMING ORGANIZATION REPORT NUMBER
UTRC - Topical Report 1990

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Defense Nuclear Agency
6801 Telegraph Road
Alexandria, VA 22310-3398
RAAE/Berggren

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
DNA-TR-90-94

11. SUPPLEMENTARY NOTES
This work was sponsored by the Defense Nuclear Agency under RDT&E RMC code B7660D SA SA 00186 RAAE 3200A 25904D.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

A preliminary analysis of the $N^* + O_2$ reaction has been carried out to predict the branching leading to the formation of vibrationally excited NO product. This analysis includes a detailed study of 31 potential energy surfaces for reactions which include all states up to $N[^2P] + O_2[X^3\Sigma_g^-]$ reactants. Only 1/6 of all collisions involving $N[^2P]$ atoms appear to lead to rovibrationally excited NO molecules. The exothermicity of the $N[^2P] + O_2$ reaction appears to mainly result in electronically excited products.

14. SUBJECT TERMS
Kinetic branching
$N^* + O_2$
Correlation diagram
$N + O_2$
Electronic state
$O + N_2$

15. NUMBER OF PAGES
22

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT
UNCLASSIFIED

18. SECURITY CLASSIFICATION OF THIS PAGE
UNCLASSIFIED

19. SECURITY CLASSIFICATION OF ABSTRACT
UNCLASSIFIED

20. LIMITATION OF ABSTRACT
SAR

CLASSIFIED BY:

N/A since UNCLASSIFIED

DECLASSIFY ON:

N/A since UNCLASSIFIED

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Conversion Table

(Conversion factors for U.S. customary to metric (SI) units of measurement)

To Convert From	To	Multiply By
angstrom	meters (m)	1.000 000 x E-10
atmosphere (normal)	kilo pascal (kPa)	1.013 25 x E+2
bar	kilo pascal (kPa)	1.000 000 x E+2
barn	meter^2 (m^2)	1.000 000 x E-28
British thermal unit (thermochemical)	joule (J)	1.054 350 x E+3
cal (thermochemical)/cm^2	mega joule/m^2 (MJ/m^2)	4.184 000 x E-2
calorie (thermochemical)	joule (J)	4.184 000
calorie (thermochemical)/g	joule per kilogram (J/kg)	4.184 000 x E+3
curie	giga becquerel (GBq)	3.700 000 x E+1
degree Celsius	degree kelvin (K)	$t_K = t_C + 273.15$
degree (angle)	radian (rad)	1.745 329 x E-2
degree Fahrenheit	degree kelvin (K)	$t_K = (t_F + 459.67)/1.8$
electron volt	joule (J)	1.602 19 x E-19
erg	joule (J)	1.000 000 x E-7
erg/second	watt (W)	1.000 000 x E-7
foot	meter (m)	3.048 000 x E-1
foot-pound-force	joule (J)	1.355 818
gallon (U.S. liquid)	meter^3 (m^3)	3.785 412 x E-3
inch	meter (m)	2.540 000 x E-2
jerk	joule (J)	1.000 000 x E+9
joule/kilogram (J/kg) (radiation dose absorbed)	gray (Gy)	1.000 000
kilotons	terajoules	4.183
kip (1000 lbf)	newton (N)	4.448 222 x E+3
kip/inch^2 (ksi)	kilo pascal (kPa)	6.894 757 x E+3
ktap	newton-second/m^2 (N-s/m^2)	1.000 000 x E+2
micron	meter (m)	1.000 000 x E-6

Conversion Table (Concluded)

To Convert From	To	Multiply By
mil	meter (m)	2.540 000 x E-5
mile (international)	meter (m)	1.609 344 x E+3
ounce	kilogram (kg)	2.834 952 x E-2
pound-force (lbf avoirdupois)	newton (N)	4.448 222
pound-force inch	newton-meter (N•m)	1.129 848 x E-1
pound-force/inch	newton/meter (N/m)	1.751 268 x E+2
pound-force/foot^2	kilo pascal (kPa)	4.788 026 x E-2
pound-force/inch^2 (psi)	kilo pascal (kPa)	6.894 757
pound-mass (lbm avoirdupois)	kilogram (kg)	4.535 924 x E-1
pound-mass-foot^2 (moment of inertia)	kilogram-meter^2 (kg•m^2)	4.214 011 x E-2
pound-mass/foot^3	kilogram-meter^3 (kg/m^3)	1.601 846 x E+1
rad (radiation dose absorbed)	gray (Gy)	1.000 000 x E-2
roentgen	coulomb/kilogram (C/kg)	2.579 760 x E-4
shake	second (s)	1.000 000 x E-8
slug	kilogram (kg)	1.459 390 x E+1
torr (mm Hg, 0°C)	kilo pascal (kPa)	1.333 22 x E-1

TABLE OF CONTENTS

LIST OF ILLUSTRATIONS

LIST OF TABLES

SECTION I

KINETIC BRANCHING OF THE $N^* + O_2$ REACTION

A study of the atmospheric reactions $O + N_2$ and $N + O_2$ which yield vibrationally excited NO molecules has been initiated. The sources of NO emission in the IR are not fully understood and the detailed kinetic branching of these reactions is being studied (References 1 and 2). In particular, the role of the $N[^2P] + O_2[X^3\Sigma_g^-]$ reaction in the production of vibrationally excited NO molecules is being examined. The current NORSE code assumes that all of the exothermicity of this reaction goes into vibrational excitation of the NO product molecule, with all levels being equally populated up to $v = 26$. The purpose of this report is to examine in detail the kinetic routes of the $N + O_2$ reaction, including those which lead to electronic as well as vibrationally excited products. A preliminary *ab initio* study of the reaction has been carried out which suggests that only a fraction of the collisions result in vibrational excitation in the product channels.

The molecular correlation diagram for the $N + O_2$ reaction is given in Table 1 for C_s, C_{2v} and $C_{\infty v}$ symmetry. This corresponds, respectively, to oblique, perpendicular and linear collisions of the N atom with the O_2 target molecule. The adiabatic molecular correlations for $C_{\infty v}$ and C_s symmetry are shown in Figs. 1 and 2, respectively. These diagrams represent a more complete version of those given by Donovan and Husain (Reference 3) and by Schofield (Reference 4).

Since the kinetic behavior is governed by an average over all collisional trajectories, we illustrate the adiabatic correlations in C_s symmetry for the doublet surfaces in Fig. 3, and for the quartet surfaces in Fig. 4. In particular, we illustrate the adiabatic connections from $N[^2P] + O_2[X^3\Sigma_g^-]$ in bold lines on these figures. The energetics of the adiabatic reaction surfaces arising from $N[^2P] + O_2$ and $N[^2D] + O_2$ are shown in Tables 2 and 3, respectively. For $N[^2P] + O_2$, only the third reaction [yielding $NO(X^2\Pi) + O^*(^1D)$] is exothermic enough to yield NO with a significant degree of vibrational excitation, provided that this reaction proceeds along an adiabatic pathway. However, there is spectroscopic evidence that curve-crossing and non-adiabatic behavior may occur for this system. The ground $^2A_1$ state of NO_2 adiabatically correlates to the reactants: $N[^4S] + O_2[X^3\Sigma_g^-]$, whereas the first excited $^2B_1$ state correlates to excited state reactants, $N[^2D] + O_2[X^3\Sigma_g^-]$. However, the $^2B_1$ state lies lower as we connect to the $NO(X^2\Pi) + O[^3P]$ dissociation limit. In addition, Gilmore (Reference 5) has pointed out that NO quenching of both $O^*[^1S]$ and $O^*[^1D]$ proceeds very rapidly, further indicating curve-crossings in the doublet surfaces.

In order to clarify the branching kinetics of the $N^*[^2P] + O_2[X^3\Sigma_g^-]$ reaction, we have initiated an extensive series of calculations of the potential energy reaction surfaces for NO_2 in the following symmetries: $^2A'$, $^2A''$, $^4A'$, $^4A''$. Preliminary CI calculations, using the GAMESS code (Reference 6), were carried out in C_s symmetry assuming a frozen core of $(1a'^2)\,(2a'^2)\,(3a'^2)$

$(4a'^2)$, $(5a'^2)$ $(6a'^2)$, which is the Hartree–Fock representation of the inner 1s and 2s electrons. Unfortunately, the characteristic charge density corresponding to this core representation differs significantly for different spin and spatial couplings of $N + O_2$. The characteristic charge of the $(6a'^2)$ pair, for example, differs in calculations in ${}^2A'$ symmetry as compared with ${}^2A''$ or ${}^4A'$ symmetry. Thus only a frozen inner shell (1s electrons) appears to be possible for this system. This smaller frozen core representation results in a great increase in the CI size, from 3048 to 28503 for ${}^2A'$ symmetry and from 3000 to 28125 for ${}^2A''$ symmetry. The calculations must therefore be carried out on a CRAY computer and the necessary code modifications for running this problem on the DNA access machines at LANL have been made. The calculations are carried out in C_s symmetry since we need to simultaneously examine the $N + O_2$ reaction path on nineteen surfaces in ${}^2A'$ and ${}^2A''$ symmetry and on twelve surfaces in ${}^4A'$ and ${}^4A''$ symmetry.

The results of our initial studies of the long range $N + O_2$ behavior are summarized in Table 4. We find that two of the states correlating to $N[^2P] + O_2[X^3\Sigma_g^-]$, ${}^2A'X$ and $2A''$ IX, exhibit long range repulsion and thus should correlate adiabatically to $NO[a^4\Pi] + O[^3P]$ and $NO[X^2\Pi] + O[^1S]$ respectively. This leaves only the ${}^2A''$ VIII surface correlating to $NO[X^2P] + O[^1D]$. For the quartet surfaces which adiabatically correlate to $NO[a^4\Pi] + O[^3P]$, no vibrationally excited ground state $NO[X^2\Pi]$ is predicted. Detailed calculations of these quartet surfaces are in progress.

The statistical branching in the $N + O_2$ reaction can be partially analyzed in terms of these calculated potential energy surfaces. In Table 2, which lists the $N^*[^2P] + O_2$ reaction surfaces, we see that only the third reaction, which yields $NO[X^2\Pi] + O[^1D]$, is exothermic enough to yield NO with any significant degree of vibrational excitation. The reaction surfaces for $N^*[^2D] + O_2$ are listed in Table 3. Three surfaces represent closed (endothermic) channels for low energy collisions and are non-reactive for air chemistry. Six surfaces produce ground state NO with nearly 4 eV internal (rovibrational) energy and one surface produces NO with less than 2 eV internal energy. Thus, of the 16 potential surfaces governing the $N[^2D] + O_2$ and $N[^2P] + O_2$ reactions, we find the following:

a. 3 are non-reactive (endothermic)

b. 6 lead to electronically excited products with the result that the NO that is produced is not rovibrational excited.

c. 7 lead to the production of ground state NO with significant (3–4 eV) rovibrational excitation.

Further, 60% of all collisions involving N[^{2}D] atoms should produce NO with significant internal excitation but only 1/6 of all collisions involving N[^{2}P] atoms appear to lead to rovibrationally excited NO molecules. Non-adiabatic behavior at closer internuclear separations could modify these relative branching ratios but will not change the conclusion that ~ 1/2 of all collisions of N[^{2}D, ^{2}P] + O_2 lead to NO with little or no rovibrational excitation. Detailed studies of these reaction surfaces are in progress to further analyze the branching rates in this system.

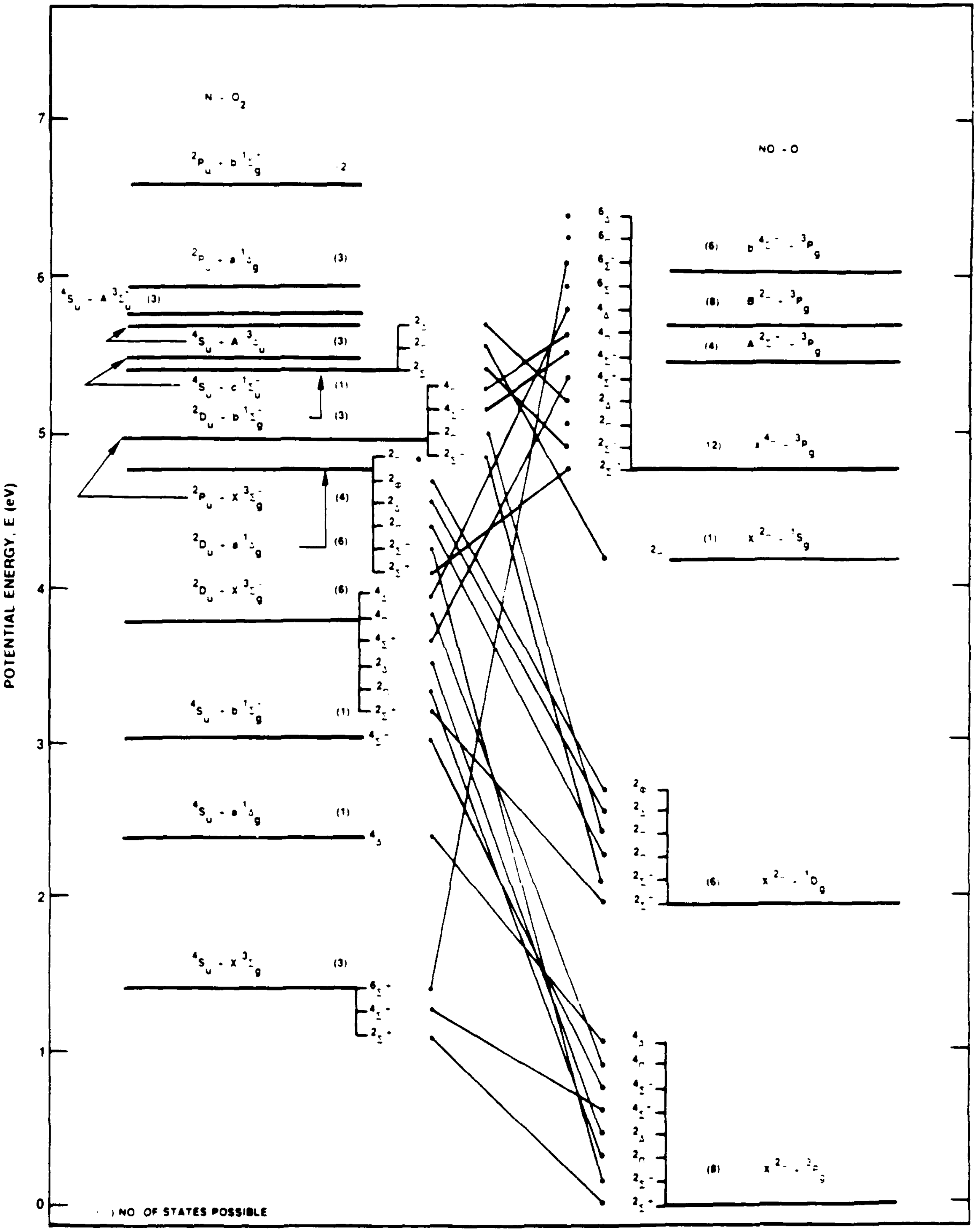

Figure 1. Molecular correlation diagram for low-lying states of NO_2 in $C_{\infty v}$ symmetry.

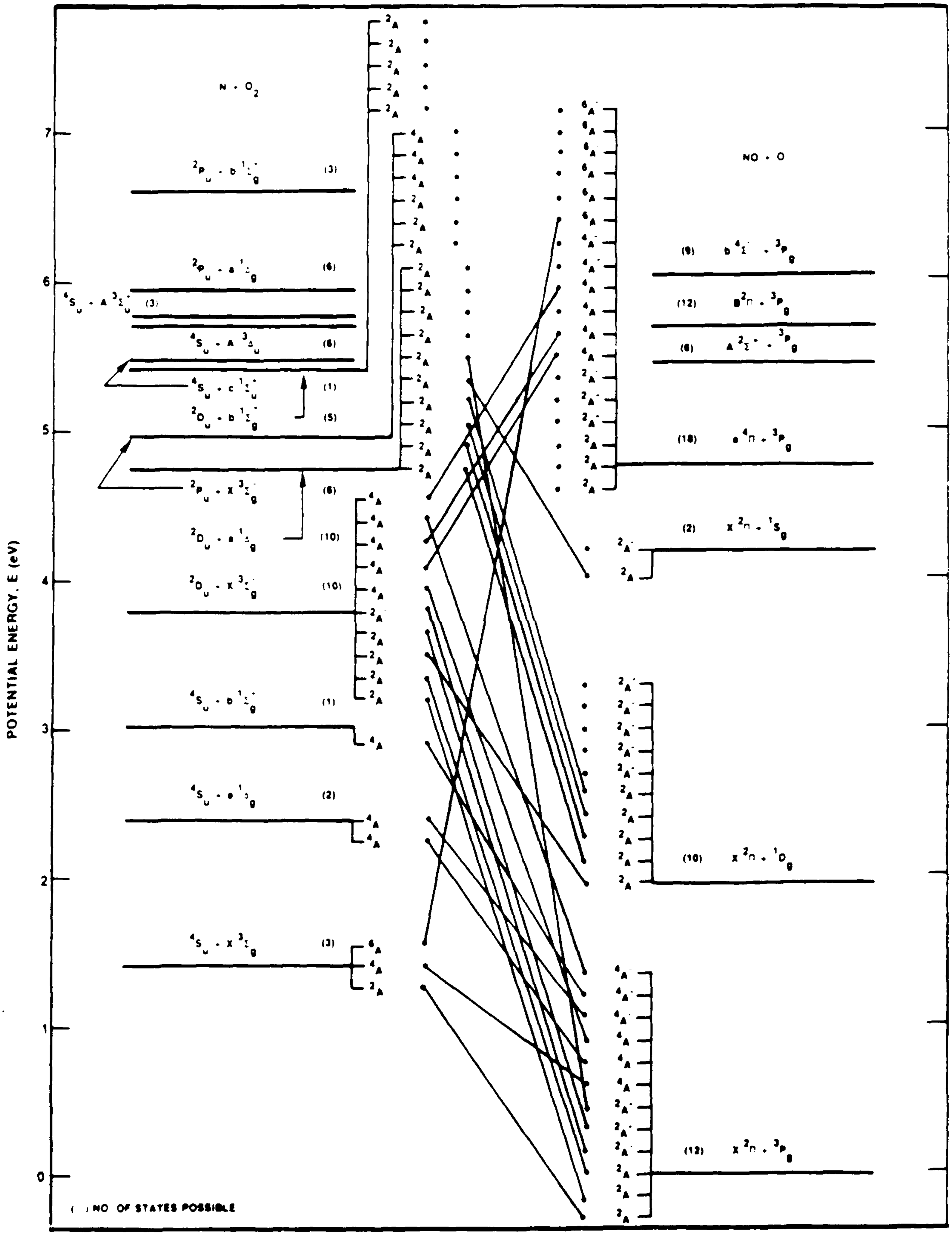

Figure 2. Molecular correlation diagram for low-lying states of NO_2 in C_s symmetry.

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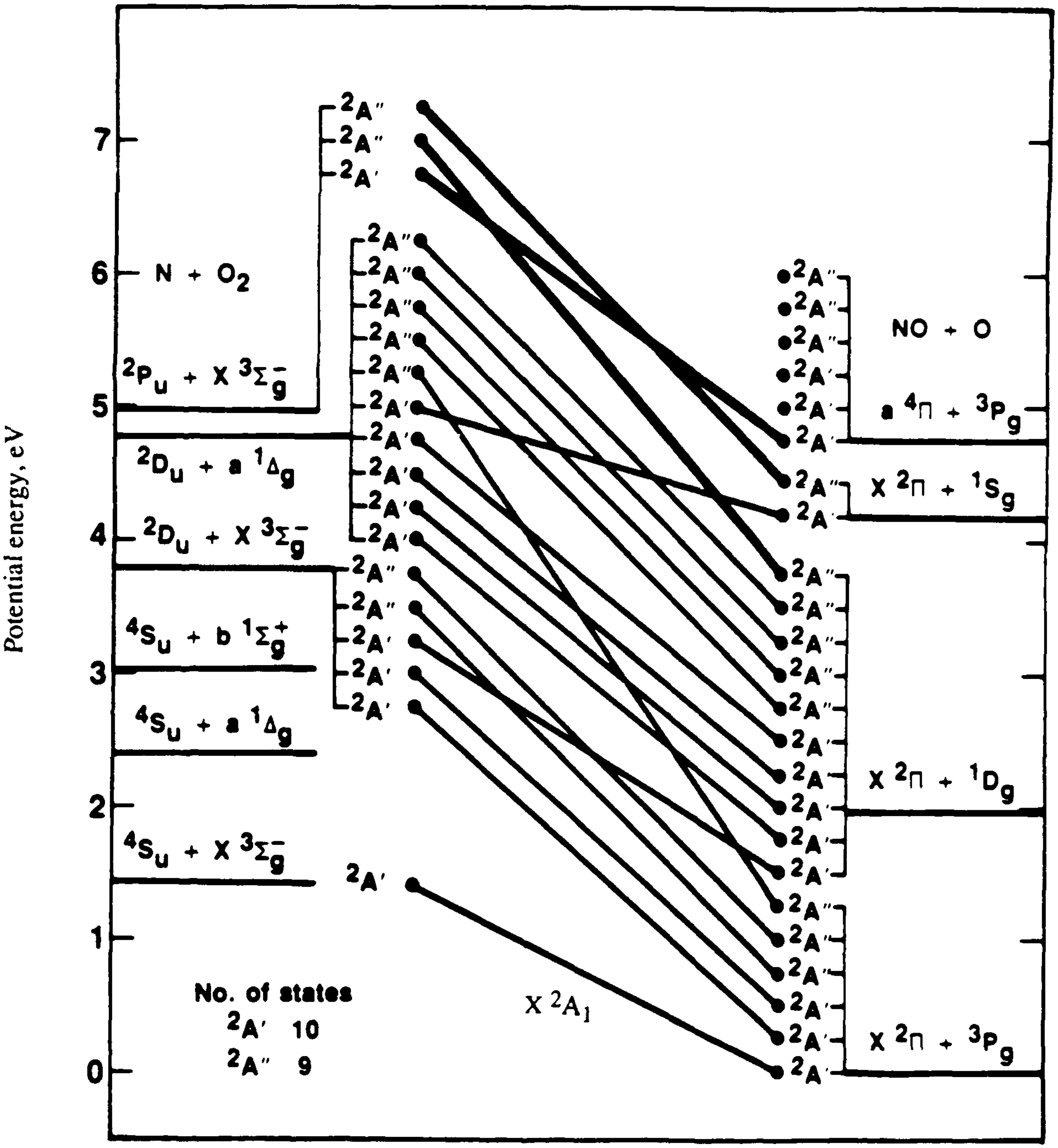

Figure 3. Molecular correlation diagram for low-lying doublet states of NO_2 in C_s symmetry.

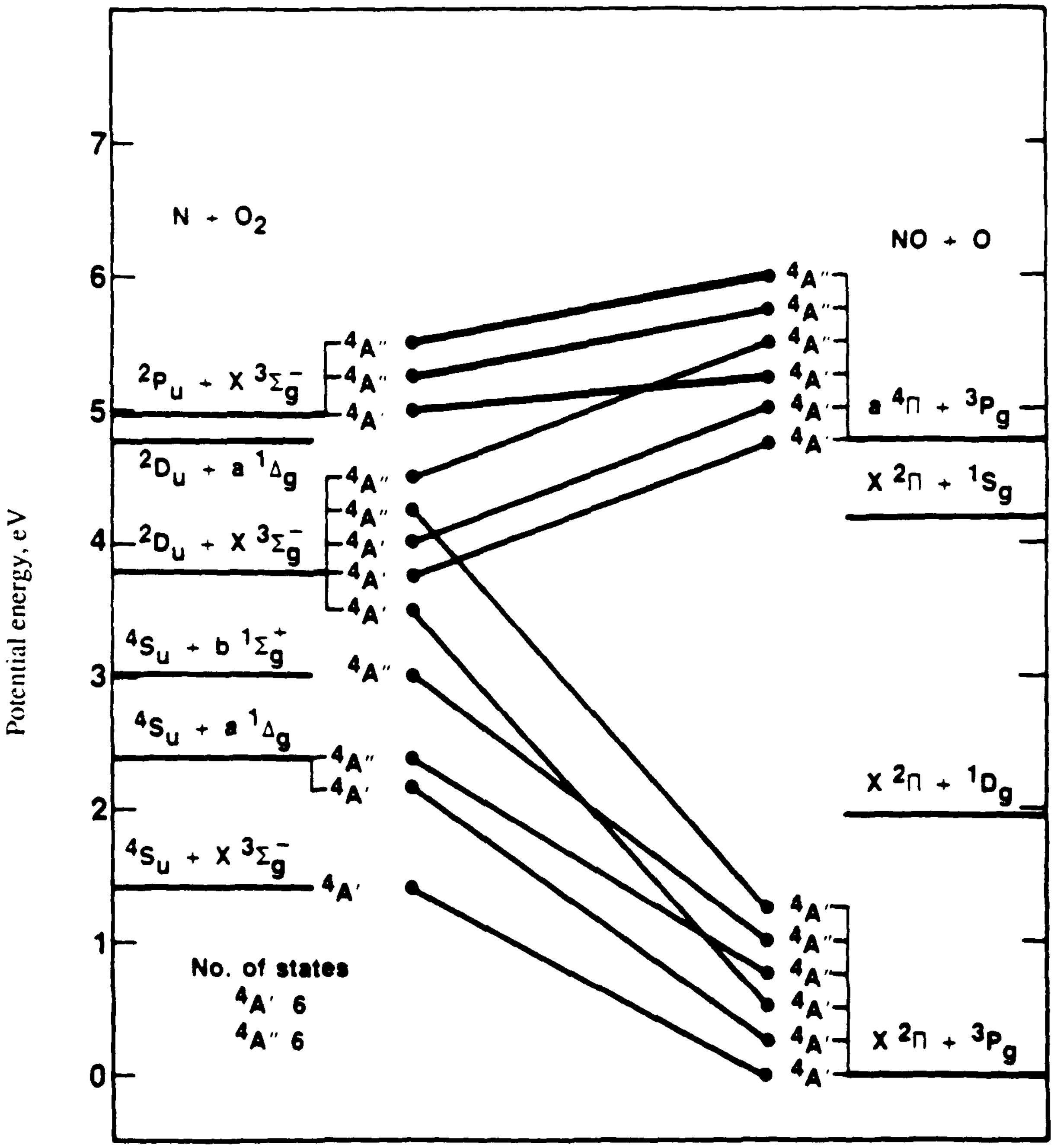

Figure 4. Molecular correlation diagram for low-lying quartet states of NO_2 in C_s symmetry.

Table 1. Molecular correlation diagram for N + O_2.

Reactants	Energy (eV)	States	Point Group
$N(^4S_u) + O_2 (X^3\Sigma_g^-)$	1.401	$^{2,4,6}\Sigma^+$	$C_{\infty v}$
		$^{2,4,6}B_1$	C_{2v}
		$^{2,4,6}A'$	C_s
$N(^4S_u) + O_2 (a^1\Delta_g)$	2.383	$^4\Delta$	$C_{\infty v}$
		$^4A_2, {}^4B_1$	C_{2v}
		$^4A'', {}^4A'$	C_s
$N(^4S_u) + O_2 (b^1\Sigma_g^+)$	3.037	$^4\Sigma^-$	$C_{\infty v}$
		$^4A_2$	C_{2v}
		$^4A''$	C_s
$N(^2D_u) + O_2(X^3\Sigma_g^-)$	3.785	$^{2,4}\Sigma^+, {}^{2,4}\Pi, {}^{2,4}\Delta$	$C_{\infty v}$
		$^{2,4}B_1$ (2), $^{2,4}B_2, {}^{2,4}A_2, {}^{2,4}A_1$,	C_{2v}
		$^{2,4}A''$ (2), $^{2,4}A'$ (3)	C_s
$N(^2D_u) + O_2(a^1\Delta_g)$	4.766	$^2\Sigma^+, {}^2\Sigma^-, {}^2\Pi, {}^2\Delta, {}^2\Phi, {}^2\Gamma$	$C_{\infty v}$
		$^2A_1$ (2), $^2A_2$ (3), $^2B_1$ (3), $^2B_2$ (2),	C_{2v}
		$^2A'$ (5), $^2A''$ (5)	C_s
$N(^2P_u) + O_2(X^3\Sigma_g^-)$	4.977	$^{2,4}\Sigma^-, {}^{2,4}\Pi$	$C_{\infty v}$
		$^{2,4}A_1, {}^{2,4}A_2, {}^{2,4}B_2$	C_{2v}
		$^{2,4}A', {}^{2,4}A''$ (2)	C_s
$N(^2D_u) + O_2 (b^1\Sigma_g{}^+)$	5.420	$^2\Sigma^-, {}^2\Pi, {}^2\Delta$	$C_{\infty v}$
		$^2A_1, {}^2A_2$(2), $^2B_1, {}^2B_2$	C_{2v}
		$^2A'$ (2), $^2A''$ (3)	C_s
$N(^4S_u) + O_2 (c^1\Sigma_u^-)$	5.499	$^4\Sigma^+$	$C_{\infty v}$
		$^4A_1$	C_{2v}
		$^4A'$	C_s
$N(^4S_u) + O_2 (A'\ ^3\Delta_u)$	5.701	$^{2,4,6}\Delta$	$C_{\infty v}$
		$^{2,4,6}A_1, {}^{2,4,6}B_2$	C_{2v}
		$^{2,4,6}A', {}^{2,4,6}A''$	C_s
$N(^4S_u) + O_2 (A^3\Sigma_u{}^+)$	5.789	$^{2,4,6}\Sigma^-$	$C_{\infty v}$
		$^{2,4,6}B_2$	C_{2v}
		$^{2,4,6}A''$	C_s

Table 1. Molecular correlation diagram for N + O_2. (Concluded)

Reactants	Energy (eV)	States	Point Group
N(^2P_u) + O_2 ($a^1\Delta_g$)	5.958	$^2\Pi$, $^2\Delta$, $^2\Phi$ $^2A_1$(2), $^2A_2$, $^2B_1$, $^2B_2$ (2) $^2A'$ (3), $^2A''$ (3)	$C_{\infty v}$ C_{2v} C_s
N(^2P_u) + O_2 ($b^1\Sigma_g^+$)	6.612	$^2\Sigma^+$, $^2\Pi$ $^2A_1$, $^2B_1$, $^2B_2$ $^2A'$ (2), $^2A''$	$C_{\infty v}$ C_{2v} C_s
Products	**Energy (eV)**	**States**	**Point Group**
NO($^2\Pi$) + O(^3P_g)	0	$^{2,4}\Sigma^+$, $^{2,4}\Sigma^-$, $^{2,4}\Pi$, $^{2,4}\Delta$ $^{2,4}A'$(3), $^{2,4}A''$(3)	$C_{\infty v}$ C_s
NO($^2\Pi$) + O (^1D_g)	1.967	$^2\Sigma^+$, $^2\Sigma^-$, $^2\Pi$(2), $^2\Delta$, $^2\Phi$ $^2A'$ (5), $^2A''$ (5)	$C_{\infty v}$ C_s
NO($^2\Pi$) + O (^1S_g)	4.189	$^2\Pi$ $^2A'$, $^2A''$	$C_{\infty v}$ C_s
NO ($a^4\Pi$) + O (^3P_g)	4.765	$^{2,4,6}\Sigma^+$, $^{2,4,6}\Sigma^-$, $^{2,4,6}\Pi$, $^{2,4,6}\Delta$ $^{2,4,6}A'$ (3), $^{2,4,6}A''$ (3)	$C_{\infty v}$ C_s
NO ($A^2\Sigma^+$) + O (^3P_g)	5.450	$^{2,4}\Sigma^-$, $^{2,4}\Pi$ $^{2,4}A'$, $^{2,4}A''$ (2)	$C_{\infty v}$ C_s
NO ($B^2\Pi$) + O (^3P_g)	5.693	$^{2,4}\Sigma^+$, $^{2,4}\Sigma^-$, $^{2,4}\Pi$, $^{2,4}\Delta$ $^{2,4}A'$ (3), $^{2,4}A''$ (3)	$C_{\infty v}$ C_s
NO ($b^4\Sigma^-$) + O (^3P_g)	6.0344	$^{2,4,6}\Sigma^+$, $^{2,4,6}\Pi$ $^{2,4,6}A'$ (2), $^{2,4,6}A''$	$C_{\infty v}$ C_s

Table 2. Adiabatic reaction surfaces arising from $N[^2P] + O_2$.

$$\begin{aligned}
N^*[^2P] + O_2[X^3\Sigma_g^-] \quad & \rightarrow NO_2^*[^2A'\ X] \rightarrow NO^*[a^4\Pi] + O\ [^3P] + 0.212\ \text{eV}\\
& \rightarrow NO_2^*[^4A'\ VI] \rightarrow NO^*[a^4\Pi] + O\ [^3P] + 0.212\ \text{eV}\\
& \rightarrow NO_2^*[^2A''\ VIII] \rightarrow NO\ [X^2\Pi] + O^*[^1D] + 3.010\ \text{eV}\\
& \rightarrow NO_2^*[^4A''\ V] \rightarrow NO^*[a^4\Pi] + O\ [^3P] + 0.212\ \text{eV}\\
& \rightarrow NO_2^*[^2A''\ IX] \rightarrow NO\ [X^2\Pi] + O^*[^1S] + 0.788\ \text{eV}\\
& \rightarrow NO_2^*[^4A''\ VI] \rightarrow NO^*[a^4\Pi] + O\ [^3P] + 0.212\ \text{eV}
\end{aligned}$$

Table 3. Adiabatic reaction surfaces arising from $N[^2D] + O_2$.

$$\begin{aligned}
N^*[^2D] + O_2[X^3\Sigma_g^-] \quad & \rightarrow NO_2^*[^2A'\ II] \rightarrow NO\ [X^2\Pi] + O\ [^3P] + 3.785\ \text{eV}\\
& \rightarrow NO_2^*[^2A'\ III] \rightarrow NO\ [X^2\Pi] + O\ [^3P] + 3.785\ \text{eV}\\
& \rightarrow NO_2^*[^2A'\ IV] \rightarrow NO\ [X^2\Pi] + O^*[^1D] + 1.878\ \text{eV}\\
& \rightarrow NO_2^*[^2A''\ I] \rightarrow NO\ [X^2\Pi] + O\ [^3P] + 3.785\ \text{eV}\\
& \rightarrow NO_2^*[^2A''\ II] \rightarrow NO\ [X^2\Pi] + O\ [^3P] + 3.785\ \text{eV}\\
& \rightarrow NO_2^*[^4A'\ III] \rightarrow NO\ [X^2\Pi] + O\ [^3P] + 3.785\ \text{eV}\\
& \rightarrow NO_2^*[^4A'\ IV] \rightarrow NO^*[a^4\Pi] + O\ [^3P] - 0.980\ \text{eV}\\
& \rightarrow NO_2^*[^4A'\ V] \rightarrow NO^*[a^4\Pi] + O\ [^3P] - 0.980\ \text{eV}\\
& \rightarrow NO_2^*[^4A''\ III] \rightarrow NO\ [X^2\Pi] + O\ [^3P] + 3.785\ \text{eV}\\
& \rightarrow NO_2^*[^4A''\ IV] \rightarrow NO^*[a^4\Pi] + O\ [^3P] - 0.980\ \text{eV}
\end{aligned}$$

Table 4. Minimum energy long range interaction potentials for $N + O_2$ in C_s symmetry.

$^2A'$	R = 4.0 bohrs[a]	R = 3.0 bohrs	Long Range Character
$^4S_u + X^3\Sigma_g^-$	-201.4657103	-201.4657669	a
$^2D_u + X^3\Sigma_g^-$	-201.3423547	-201.3428036	a
	-201.3423540	-201.342542	r
	-201.3423535	-201.3415228	r
$^2D_u + a^1\Delta_g$	-201.3045858	-201.3051402	a
	-201.3045827	-201.3048667	a
	-201.3045808	-201.3043220	r
	-201.3045790	-201.3041826	r
	-201.3045775	-201.3040453	r
$^2P_u + X^3\Sigma_g^-$	-201.2994959	-201.2988189	r
$^2A''$			
$^2D_u + X^3\Sigma_g^-$	-201.3423546	-201.3427958	a
	-201.3423536	-201.3420978	r
$^2D_u + a^1\Delta_g$	-201.3045845	-201.3051136	a
	-201.3045830	-201.3048777	a
	-201.3045810	-201.3043588	r
	-201.3045790	-201.3041614	r
	-201.3045775	-201.3040561	a
$^2P_u + X^3\Sigma_g^-$	-201.2994986	-201.2999683	a
	-201.2994921	-201.2987603	r

[a] R is measured from N to the center of the O_2 molecule, energy in hartrees.

SECTION 2

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