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We have investigated intermediates and products in the thermal decomposition of RDX vapor, using a variety of experimental microwave techniques previously employed in our laboratory in studies of pyrolysis decomposition of organic amines. We used microwave spectroscopy to determine the chemical composition of the decomposition of nitramines by pyrolysis methods and identify the products in the thermal decomposition processes. The objective was to determine the validity of proposed decomposition mechanisms, and to identify new reaction products or pathways.

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THERMAL DECOMPOSITION PATHWAYS IN NITRAMINE PROPELLANTS

FINAL REPORT

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# THERMAL DECOMPOSITION PATHWAYS IN NITRAMINE PROPELLANTS

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## Abstract

We have investigated intermediates and products in the thermal decomposition of RDX vapor, using a variety of experimental microwave techniques previously employed in our laboratory in studies of pyrolysis decomposition of organic amines. We used microwave spectroscopy to determine the chemical composition of the decomposition of nitramines by pyrolysis methods and identify the products in the thermal decomposition processes. The objective was to determine the validity of proposed decomposition mechanisms, and to identify new reaction products or pathways.

## I. Background

Nitramine propellants<sup>1</sup> are energetic chemical compounds containing nitro groups chemically bound to other nitrogen atoms, i.e., containing fragments of the form N-NO<sub>2</sub>. RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine) and HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazine) are two of the most widely used propellants of this type, and considerable research exists on the macroscopic ignition and combustion properties of RDX and HMX<sup>2-7</sup>. In order to optimize the application of explosives such as RDX and HMX, as well as to devise improved propellants with related chemical properties, a knowledge of the microscopic ignition and combustion behavior of these propellants is required. Obtaining molecular level information on nitramine ignition and combustion in the high-pressure, high-temperature environments typical of actual propellant applications is not easy. It therefore makes sense to pursue an alternative strategy of obtaining information under more controlled laboratory conditions, and transferring this information to the harsher application

environments. We have employed microwave spectroscopy to determine with certainty the chemical composition of many of the products of thermal decomposition of RDX. Thermal decomposition was induced both by simple heating of the sample in a metal nozzle and by a rather gentle thermal pyrolysis technique in which the vapor of RDX is flowed over a heated catalytic substrate.

### 1. Nitramine Combustion and Decomposition Chemistry

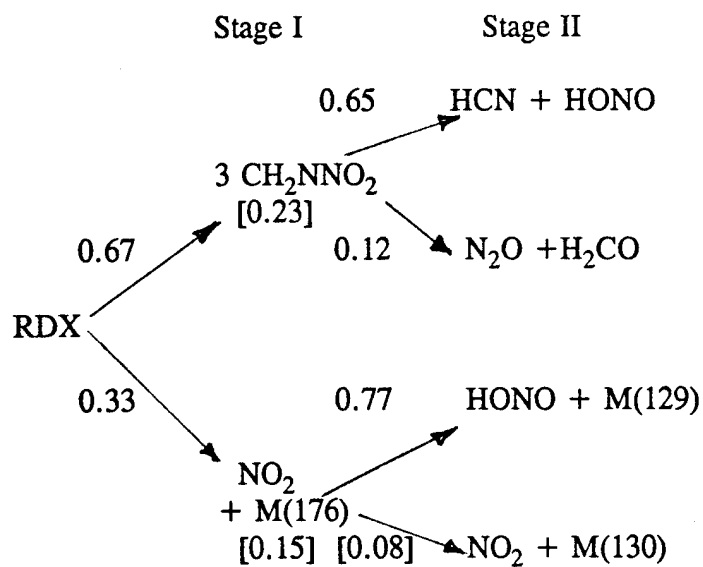
Detailed chemical kinetics mechanisms for ignition and combustion are not well known for any of the energetic propellants. Nevertheless, recent detailed chemical kinetics modelling efforts<sup>8-10</sup> have led to a global understanding for common nitramine propellants which is relatively successful. Melius<sup>8,9</sup> used a model containing 31 chemical species and 137 chemical reactions to reproduce species profiles, flame speed, and pressure dependence for a 0.05 MPa RDX flame. The success of this model suggests that efforts to make it more complete are desirable, and it is in this context that the present study of the chemical composition of early decomposition products should be viewed.

Zhao, Hintsas and Lee<sup>11</sup> used a time-of-flight (TOF) mass spectrometer to detect decomposition products after infrared multiphoton dissociation of RDX in a molecular beam in order to investigate the mechanism of RDX thermal decomposition. They determined photodissociation channels, branching ratios and translational energy distributions. In contrast to the conventional view before their work, i.e., the view that simple bond rupture through loss of NO<sub>2</sub> was the dominant primary channel in RDX thermal decomposition, Zhao, Hintsas and Lee found that the dominant primary channel of photodecomposition is a

concerted symmetric triple fission to produce three  $\text{CH}_2\text{N}_2\text{O}_2$  (mass 74) fragments, which subsequently undergo secondary concerted dissociation to produce HCN,  $\text{H}_2\text{CO}$ , HONO (or possibly the isomeric  $\text{HNO}_2$ ) and  $\text{N}_2\text{O}$ . A total of two primary and four secondary dissociation channels were observed.

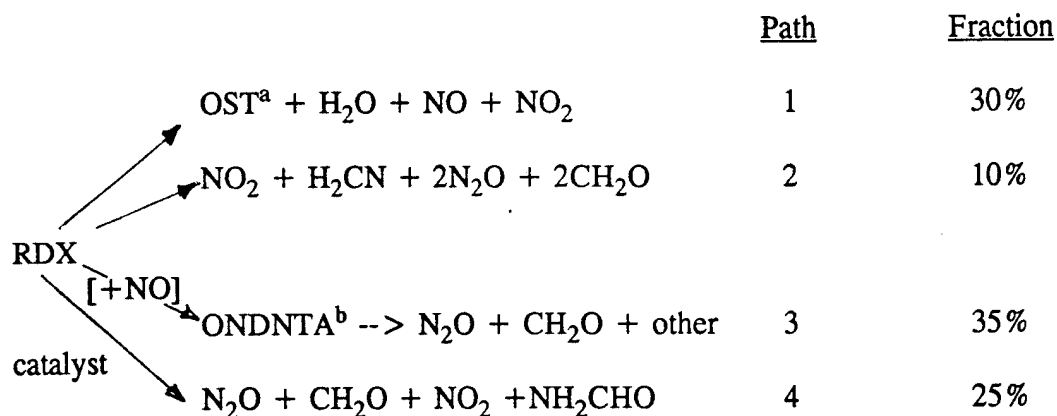
## 2. RDX Decomposition - Photolysis Versus Thermal Decomposition

The reaction scheme described above has some parallels in the unimolecular laser infrared multiphoton dissociation (IRMPD) photolysis decomposition scheme for RDX proposed by Zhao, et al.<sup>11</sup> through deconvolution of the time-of flight mass spectra which is illustrated below:



The dominant channel is a concerted triple fission of the RDX ring to produce three  $\text{CH}_2\text{N}_2\text{O}_2$  (mass 74) fragments which was identified to be the  $\text{CH}_3=\text{NNO}_2$  species. Zhao et al.<sup>11</sup> contend that the dissociation mechanism obtained in IRMPD experiments is the same as that in thermal decomposition experiments on other moderate size systems they have investigated.

Recent pyrolysis studies by Behrens<sup>12-13</sup> on RDX and HDX, which employed thermogravimetric modulated beam and time-of flight mass spectrometry, suggest that decomposition in the liquid phase differs from the gas phase IRMPD experiments. Behrens found that both nitramines form H<sub>2</sub>O, N<sub>2</sub>O, CH<sub>2</sub>O, NO and (CH<sub>3</sub>)NHCHO. In addition, RDX produces NO<sub>2</sub> and hydroxy-s-triazine from N-N bond breaking while HMX forms C<sub>2</sub>H<sub>6</sub>N<sub>2</sub>O (mass 74), CO and a residue. Behrens argues that the mass 74, with stoichiometry of C<sub>2</sub>H<sub>6</sub>N<sub>2</sub>O, is not methylenenitramine (CH<sub>2</sub>N<sub>2</sub>O<sub>2</sub>) as suggested in the IRMPD study based on deuterium and <sup>15</sup>N labelling experiments, but they do not offer a molecular formula to explain this mass peak. All conceivable structures for this species would require bimolecular reactions since the N=O bond must be ruptured or modified by atom addition. The primary species produced in the thermal decomposition studies of liquid RDX are N<sub>2</sub>O, CH<sub>2</sub>O, and H<sub>2</sub>O, while secondary products are CO, NO, and HCN with minor products C<sub>2</sub>H<sub>5</sub>NO and C<sub>2</sub>H<sub>6</sub>N<sub>2</sub>O. Behrens and Bulusu<sup>14,15</sup> propose the following decomposition paths for liquid RDX at temperatures between 195° C and 215° C:



The first and second pathways are first-order reactions in the decomposition of RDX. Based on their time-of-flight spectra, they concluded that the products HCN, N<sub>2</sub>O, HONO, NH<sub>2</sub>CHO, and C<sub>3</sub>H<sub>3</sub>N<sub>3</sub>O (oxy-s-triazine) arise only from other decomposition products. The products CO, CH<sub>2</sub>O, NO and NO<sub>2</sub> show contributions from RDX and from other decomposition products. No direct evidence for formation of CH<sub>2</sub>=NNO<sub>2</sub> was reported, and the H<sub>2</sub>CN species in pathway 2 appears to have been added to account for the chemical

balance based on the RDX formula,  $C_3H_6N_6O_6$ . Thus, the RDX decomposition experiments studied by the thermogravimetric-mass spectroscopy methods yield dramatically different results than the IRMPD studies and leave many questions unanswered. Mass spectroscopic investigations such as these are clearly an essential tool for studying the decomposition chemistry of nitramine propellants, but mass spectroscopy suffers somewhat as a detection technique from the fact that missing mass peaks, unexpected cracking patterns, complex TOF patterns, and lack of structural information on the products sometimes leads to uncertainties in the interpretation of the identification of the molecular species. It is precisely these uncertainties which might be resolved by microwave studies of the type described here.

## II. Experimental Results

The instruments employed are (a) a Stark-modulated millimeterwave spectrometer with computer controlled frequency scanning and equipped with a pyrolysis source, and (b) pulsed-beam Fabry-Perot cavity Fourier-transform microwave (FTMW) spectrometer with a heated nozzle source<sup>19</sup> shown in Figure 1. The frequency coverage of the millimeterwave spectrometer (a) is 18 GHz to 170 GHz using both solid-state and klystron frequency sources, while for the FTMW spectrometer (b) the current frequency range is 6 GHz to 26 GHz. Both spectrometers have computer controlled scan capabilities for broad-band coverage. In the millimeterwave study we used a flow pyrolysis system consisting of a 6 mm o.d. glass tube, filled with granular zeolite material (alumina-silicate) which has been found to produce pyrolytic decomposition at reduced temperatures, heated to 200°-450° C over a length of about 20 cm to study the thermal decomposition products of RDX vapor.

The RDX solid was placed in a small quartz boat 10 cm in length and heated to between 140° and 150° C by a heating tape wrapped around the glass tube surrounding the RDX sample. This system is illustrated in Figure 2a. and 2b.

## 1. Pulsed-beam Fourier-Transform Experiments

### A. Survey of RDX

We have covered the frequency range searched for decomposition products with the FTMW spectrometer with coverage of 6.6 GHz between 8-18 GHz. The RDX sample was placed in a heated reservoir of the pulsed nozzle and pressurized with Ar at 1.2 kPa. Most of the survey was carried out with nozzle temperatures between 140°C and 150°C, and covered the key regions of the known decomposition products as well as searches for methylene nitramine,  $\text{CH}_2=\text{NNO}_2$ , which is produced in the unimolecular decomposition by Zhao, *et al.*<sup>1</sup>. By far the most intense products are  $\text{H}_2\text{CO}$  and  $\text{N}_2\text{O}$ , followed by HONO,  $\text{NH}_2\text{CHO}$  (formamide) and HNCO. In addition to monomer spectra, several dimers were observed, namely  $(\text{H}_2\text{O})_2$ ,  $\text{Ar-H}_2\text{CO}$ , and  $\text{NH}_2\text{CHO-H}_2\text{O}$ , since the beam temperature is between 1-5 K. The water appears to originate in the decomposition, since it is not "baked out" of the sample. The species  $\text{H}_2\text{CO}$ ,  $\text{N}_2\text{O}$ , and  $\text{NH}_2\text{CHO}$  were sufficiently intense to allow measurement over a range in temperatures (about 140°-190°C) and each showed an exponential growth since the vapor pressure and decomposition are proportional to the temperature. Only one feature has been observed but not assigned. This occurs as a triplet near 9156.35 MHz, the carrier contains  $\text{H}_2\text{CO}$  since it is observed from a pure formaldehyde sample. A summary of the transitions detected in this survey is given in Table I. No

evidence was found for spectra from RDX or methylene nitramine.

### B. Structure of Nitromethane-Water

The stimulus for the study of the nitromethane-water complex derives from the theoretical work of Melius<sup>20,21</sup> in which water is found to exert a strong catalytic effect in reducing the barrier to the decomposition of nitramines. Examples are presented for the reactions of nitramine and nitromethane in which "water provides a concerted, cyclic reaction pathway for reduction of the nitro group."<sup>21</sup> The transition state, depicted in Fig. 1b, shows a reduction in the barriers by 27 kcal mol<sup>-1</sup>. We have studied a number of complexes in which the transition state geometry is replicated by the van der Waals complex at longer distance and strongly suggest that the complexes lie along the reaction coordinate.

Examples studied are the complexes for ozone-ethylene<sup>22</sup>, ozone-acetylene<sup>23</sup> and ketene-ethylene<sup>24</sup>; the ozone complexes exhibit cyclic van der Waals structures and ketene-ethylene has the heavy atom frames crossed at 90°. Thus, we were interested in determining the geometry the nitromethane-water with respect to the proposed cyclic transition state.

The microwave spectrum of the nitromethane-water complex has been studied with FTMW spectrometer. The dominant spectrum is *b*-type with a weaker *a*-type spectrum. Critical to the rotational assignments were well resolved <sup>14</sup>N nuclear electric quadrupole transitions, and the incorporation of the pulsed nozzle in one of the mirrors which provided a beam co-axial with the cavity axis to attain linewidths on the order of 2 kHz. In addition to the CH<sub>3</sub>NO<sub>2</sub>-H<sub>2</sub>O species, substitutions of HDO and D<sub>2</sub>O in the complex were made, and the CD<sub>3</sub>NO<sub>2</sub>-H<sub>2</sub>O species was also assigned. The molecular structure derived from the moments of

inertia, shown in Fig. 3, has the dipolar axes of each monomer nearly parallel with a center of mass separation of 3.506(7) Å. The complex is quite strongly bonded with a stretching force constant  $k_s = 9.3$  N/m and evidence for two hydrogen bonds of 2.16 Å between an O atom of the NO<sub>2</sub> group and a water H atom, and 2.09 Å between a CH<sub>3</sub> proton and the oxygen atom of water. Unpublished *Ab initio* calculations by W. J. Stevens support this structure. A report describing these results has been accepted for publication in *J. Mol. Spectrosc.*<sup>25</sup>

## 2. Pyrolysis Studies of RDX Vapor - Microwave Studies

This experiment involves a conventional microwave absorption spectrometer equipped with a pyrolysis inlet. The RDX sample is heated to a fixed temperature, typically 145° C, and the vapor passes over an alumina-silica catalyst at a higher temperature (200°-450° C) to decompose the vapor. Extensive surveys have been conducted between 54 GHz and 150 GHz with a new synthesizer-locked backwardwave oscillator source from 50-78 GHz and 78-118 GHz from the Russian firm Kvarz. We were able to frequency double the lower frequency unit to survey the region from 123.5-150 GHz. We have assigned less than 10% of these transitions to known species. As in the nozzle experiment, the dominant products are H<sub>2</sub>CO and N<sub>2</sub>O, with ground and vibrationally excited states detected. Formamide (NH<sub>2</sub>CHO) and isocyanic acid (HNCO) are observed and the latter peaks at high catalyst temperature (about 400° C), which suggests that HNCO is produced by decomposition of another product, perhaps formamide, produced at an earlier stage. Several transitions of NO, NO<sub>2</sub> and HONO are observed but are quite weak. The new survey also show more than a dozen lines of CH<sub>3</sub>OH. The methanol appears to be an impurity in the RDX sample

since its spectra grows weak the longer the RDX sample is heated, while the other products continue to show strong spectral lines. Our survey contains hundreds unidentified features, and efforts to assign these (or a subgroup of these) to the triple fission product,  $\text{CH}_2=\text{NNO}_2$ , were unsuccessful in spite of a high quality *ab initio* structure as a guide. Figure 4 shows a calculated spectrum of  $\text{CH}_2=\text{NNO}_2$  based on the *ab initio* structure<sup>26</sup> between 75 GHz and 120 GHz; this may be compared to the observed unassigned spectra over the same frequency range in Figure 4. Thus, either  $\text{CH}_2=\text{NNO}_2$  is not produced in the RDX vapor decomposition or it is not sufficiently stable to be detected under the conditions of this experiment. A summary of the observed microwave transition for the species identified is given in Table II and the unassigned lines are listed in Appendix I. Behrens and Bulusu<sup>14</sup> report N-methylformamide,  $\text{CH}_3\text{NHCHO}$  (mass 59), as a minor product based on the ion signal at  $m/z = 58$ . We have examined and assigned a portion of the millimeterwave spectrum of N-methylformamide with the aid of unpublished lower frequency measurements by R. A. Elzara (PhD Thesis Michigan State University). When comparing the same spectral region surveyed in the RDX pyrolysis, no evidence of N-methylformamide was found.

#### A. Species X - Assignment of Unidentified Species

During the course of surveying the pyrolysis products of RDX vapor, three lines with resolved Stark effect were observed between 70 GHz and 75 GHz. Each had two Stark shifted components characteristic of *a*-type  $J = 2-1$  R-branch transitions. Subsequent scans at higher harmonic frequencies for the  $J = 3-2$  and  $J = 4-3$  transitions provided additional transitions with the expected Stark effect for this assignment. Table IV lists 12 assigned

transitions for this unknown molecular species which we have labeled "Species-X". The fitted rotational constants are also shown in Table IV. We have tested Species-X by applying a strong magnetic field and see no effect on the spectral lines, thus, it is not paramagnetic and eliminates a radical as a source of the spectrum. The inertial defect,  $\Delta I$ , is small and positive, which indicates that Species-X is a planar molecule. The magnitude of the rotational constants indicates the species is light and prolate (like formaldehyde or methanol) and the assigned lines all arise from a  $\mu_a$  dipole moment component. We attempted to locate a *b*-type or *c*-type Q-branch series unsuccessfully. Species-X was observed from virtually every sample of RDX which we pyrolyzed, and also was observed in several sample of HMX pyrolyzed in the same manner as the RDX experiment. Assuming that Species-X is a product of RDX vapor decomposition, and there is no reason to believe otherwise, it is constrained to be composed of  $H_nC_xN_yO_z$  where *n*, *x*, *y*, and *z* are integers, since the empirical formula of RDX is  $C_3H_6N_6O_6$ . Further, every known species having three first row atoms (C, N or O) in any combination has B and C rotational constants near 10 to 13 GHz, much smaller than Species-X. Thus, we are led to believe that Species-X can contain only two of these first row atoms. In Table V we have constructed a chart of all pairs of C, N, and O and then adding H's until the valence bonding is saturated. At the bottom of Table V rotational constants from microwave spectral analysis are shown. From the magnitude of the A rotational constant (140 GHz) for Species-X, it is clear that 3 hydrogen atoms off the heavy atom axis ( $H_2NOH$  or  $CH_2=NH$ ) are too few and 5 hydrogen atoms are too many ( $CH_3NH_2$ ), while 4 hydrogen atoms are close ( $H_2NNH_2$  and  $CH_3OH$ ). The methylamine B and C rotational constants are slightly larger (10%) than Species-X, which is true of the

other saturated forms of the diatoms. The puzzle is in the fact that all of the stable species (radicals were not considered based on the results of the paramagnetic test) we can conceive of are listed in Table V and each of these either has no microwave spectrum ( $H_nC_2$  species) due to a lack of dipole moment, or has already been assigned, i.e. we know the rotational constants, and these do not explain Species-X. Thus, our best guess for the formula of Species-X is  $H_4XY$ , where X and Y = C, N, or O.

### B. Temperature profiles

Temperature profiles of the identified species whose intensities were sufficiently strong were measured by keeping the temperature of the RDX sample constant and increasing (or decreasing) the temperature of the catalyst pyrolysis zone. In Figure 6 profiles for HCN,  $H_2CO$ ,  $N_2O$ , CO, HNCO, and Species-X are shown. The results are rather poor due to the slow flow employed in order to maintain a constant pressure in the absorption cell. With increasing temperature the cell pressure increased due to more decomposition, while the opposite occurs when starting at the highest temperature and decreasing the temperature. However, a general trend is evident: The  $N_2O$ ,  $H_2CO$  and Species-X were strongest at pyrolysis temperatures between  $250^\circ C$  and  $300^\circ C$ , while HCN and HNCO had a peak intensity between  $400^\circ C$  and  $450^\circ C$ . The CO species was rather constant over the whole range and  $NO_2$  shows increasing intensity up to  $450^\circ C$ . Thus, it would appear that Species-X,  $H_2CO$  and  $N_2O$  appear as first stage products, while HCN and HNCO are second stage products, i.e. result from pyrolysis of first stage products. Very likely HNCO comes from pyrolysis of formamide ( $NH_2CHO$ ). These results are in agreement with those of Behrens and Bulusu<sup>14</sup>. It is interesting that species-X correlates with the first stage products.

### III. Conclusions

The unimolecular laser infrared multiphoton dissociation (IRMPD) photolysis decomposition scheme for RDX proposed by Zhao, et al.<sup>1</sup> showed that the dominant channel is a concerted triple fission of the RDX ring to produce three  $\text{CH}_2\text{N}_2\text{O}_2$  (mass 74) fragments and identified it to be the  $\text{CH}_2=\text{NNO}_2$  species. Behrens and Bulusu<sup>2</sup> have studied the decomposition of liquid RDX and several isotopically labeled species and concluded that four pathways occur in the liquid including a surface catalyzed path in which  $\text{NH}_2\text{CHO}$  is produced. Several large species were initially formed, namely, oxy-s-triazine ( $\text{C}_3\text{H}_3\text{N}_3\text{O}$ ) and 1-nitroso-3,3-dinitrohexahydro-s-triazine, whose structure and microwave spectra are unknown. The observed products in our experiments correlate better with the mechanism of Behrens and Bulusu, although several differences were found. We did not observe N-methylformamide attributed to mass peak  $m/z = 58$ , and we detected several species not reported in the mass spectrometry study, namely, Species-X,  $\text{HCOOH}$ ,  $\text{HNCO}$ , and possibly acetaldehyde,  $\text{CH}_3\text{CHO}$ . Most of the spectral lines observed in the millimeterwave survey remain unassigned. Perhaps these may be attributed to the two species detected by mass spectrometry, OST (oxy-s-triazine) and ONDNTA (1-nitroso-3,5-dinitrohexahydro-s-triazine), whose microwave spectrum is unknown. Cosgrove and Owen<sup>27</sup> reported the detection of formic acid in the decomposition of RDX vapor at  $195^\circ\text{C}$  via a chemical test. It might be noted that  $\text{HCOOH}$  has the same mass (46) as  $\text{NO}_2$  and  $\text{CH}_3\text{CHO}$  has the same mass (44) as  $\text{N}_2\text{O}$ , thus, the presence in the mass spectrum might be masked by this other known products.

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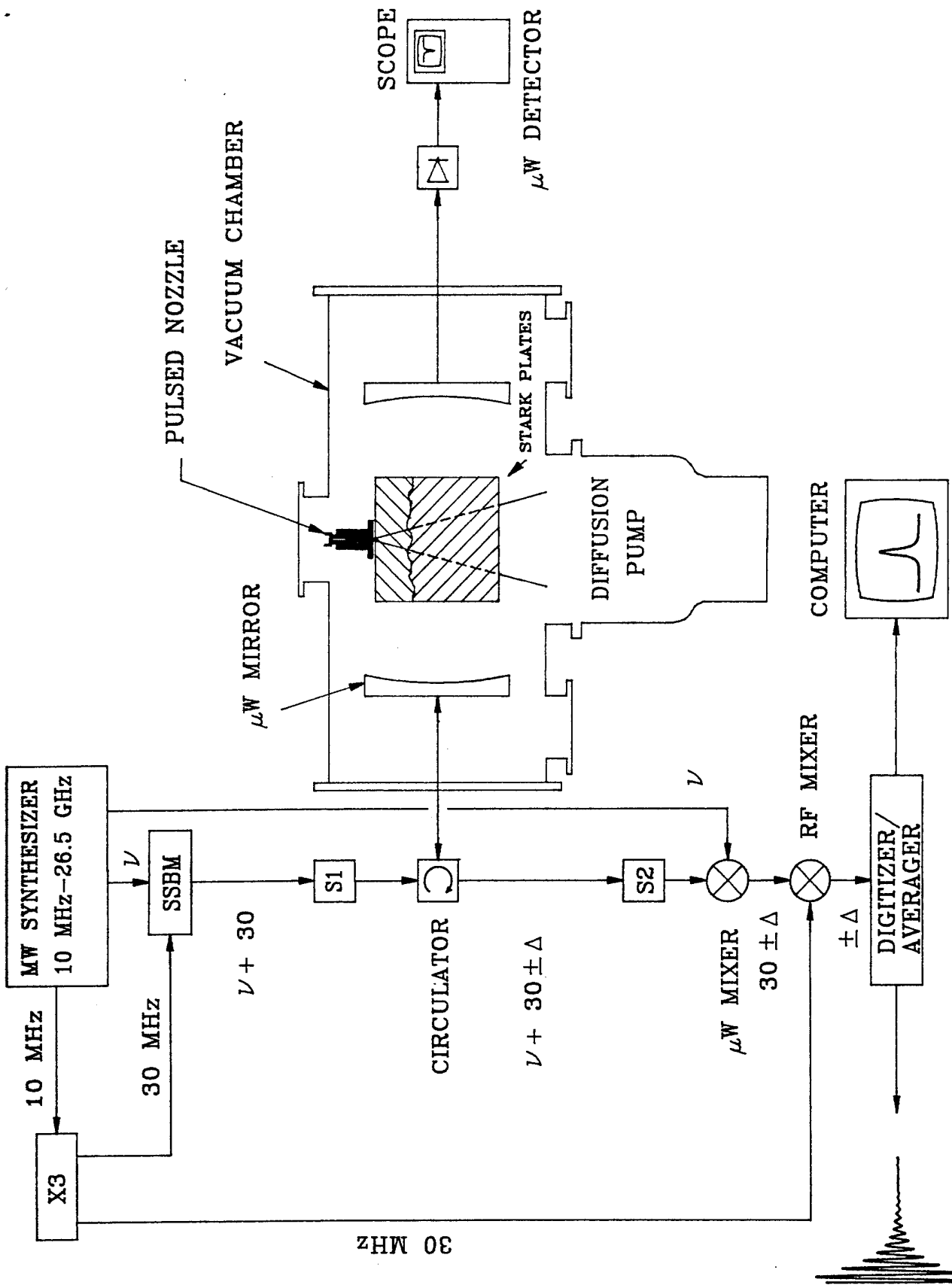
## LIST OF PUBLICATIONS

F.J. Lovas, N. Zobov, G.T. Fraser, and R.D. Suenram, *J. Mol. Spectrosc.* **171**, xxx (1995).

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# Millimeterwave Synthesizer

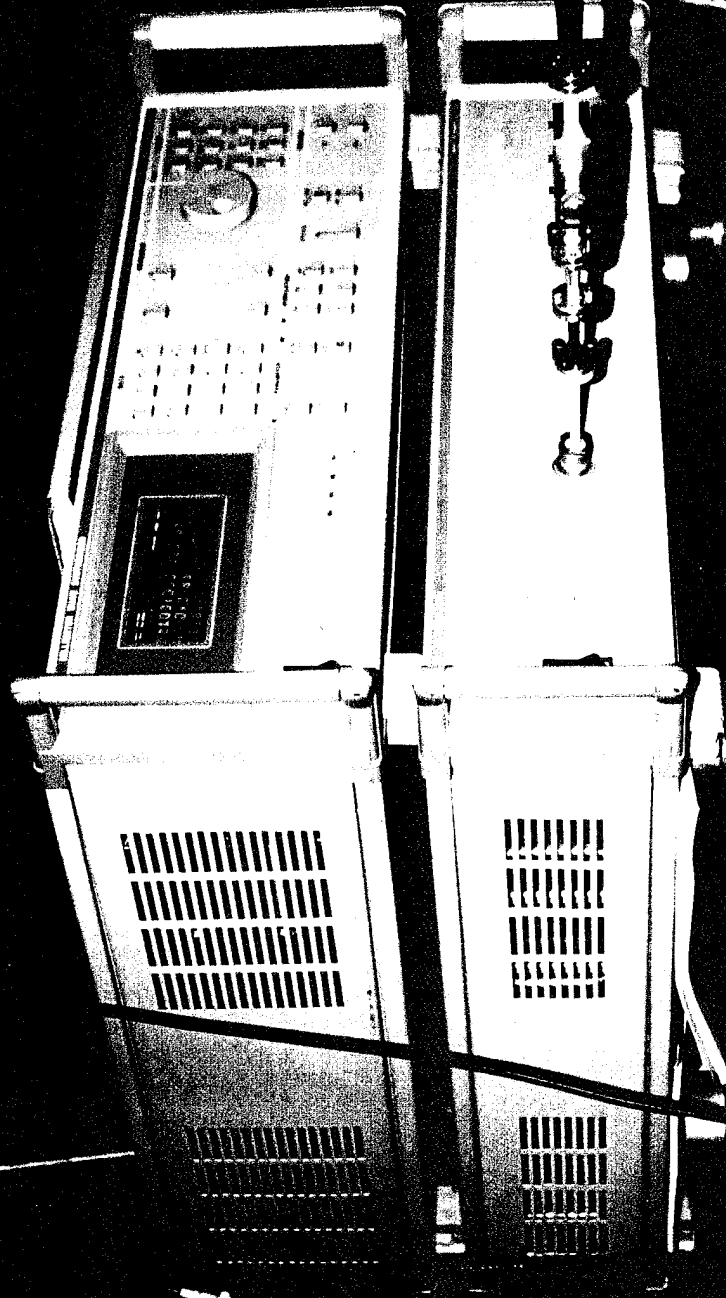
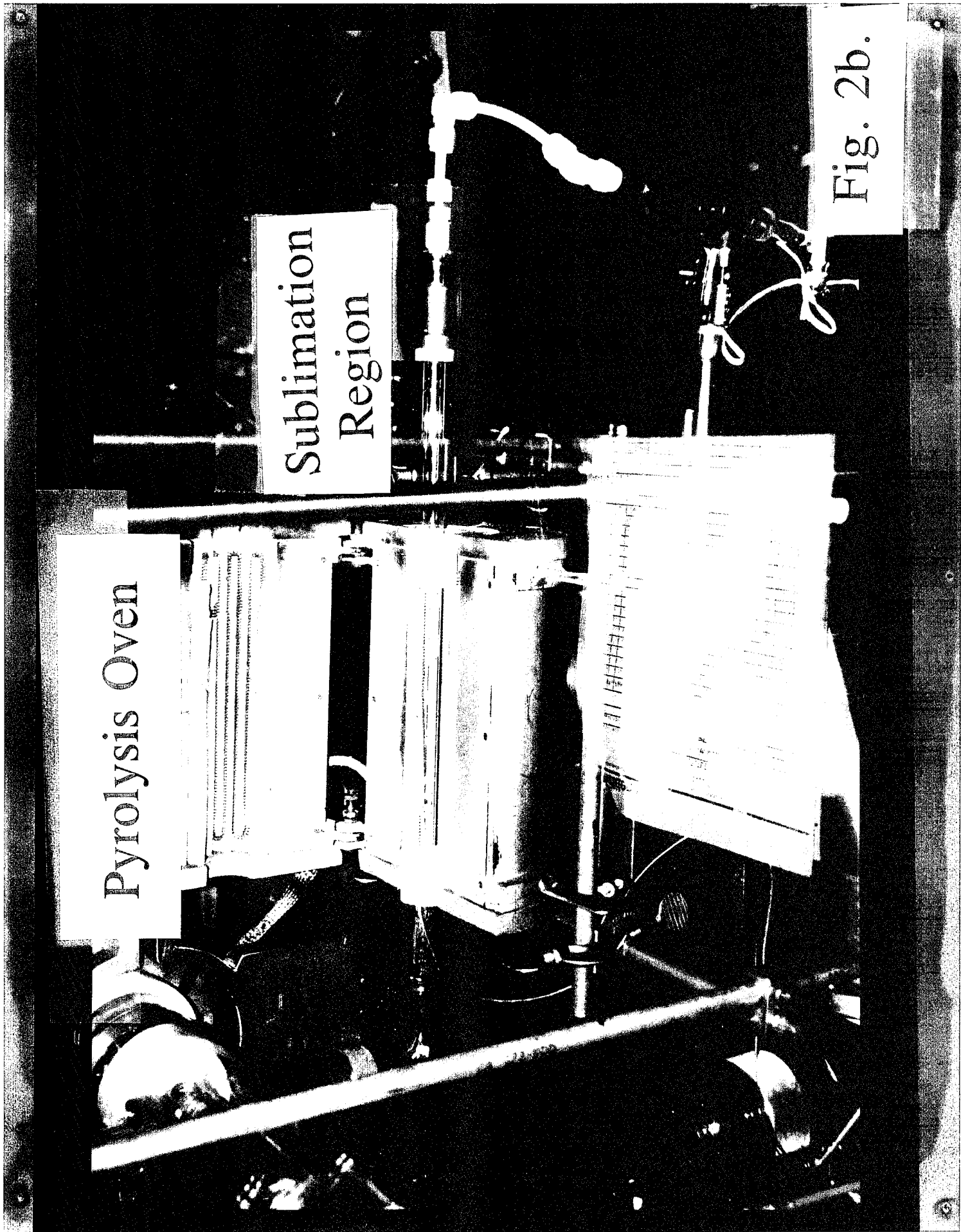


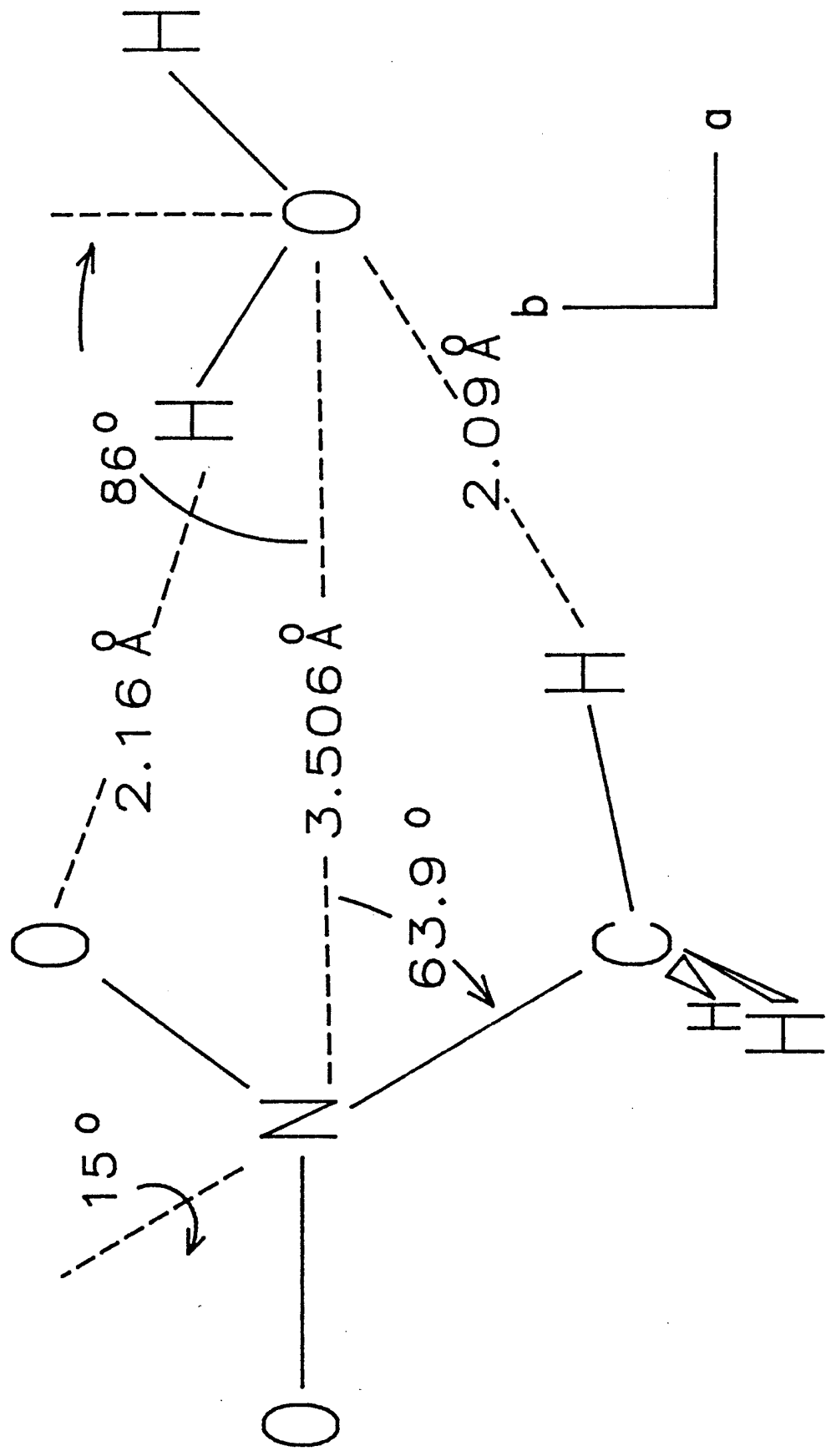
Fig. 2a.

Pyrolysis Oven

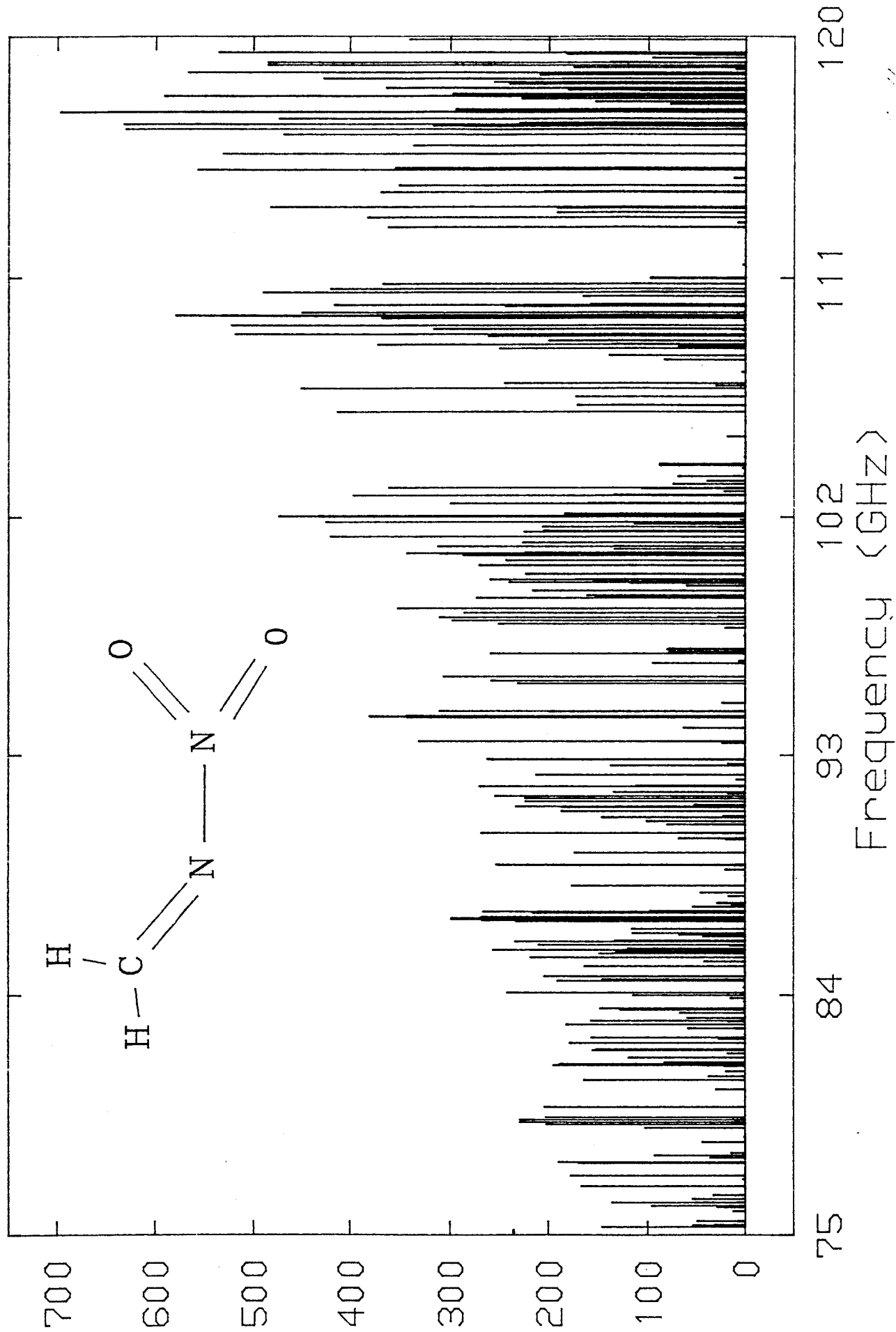
Sublimation  
Region

Fig. 2b.

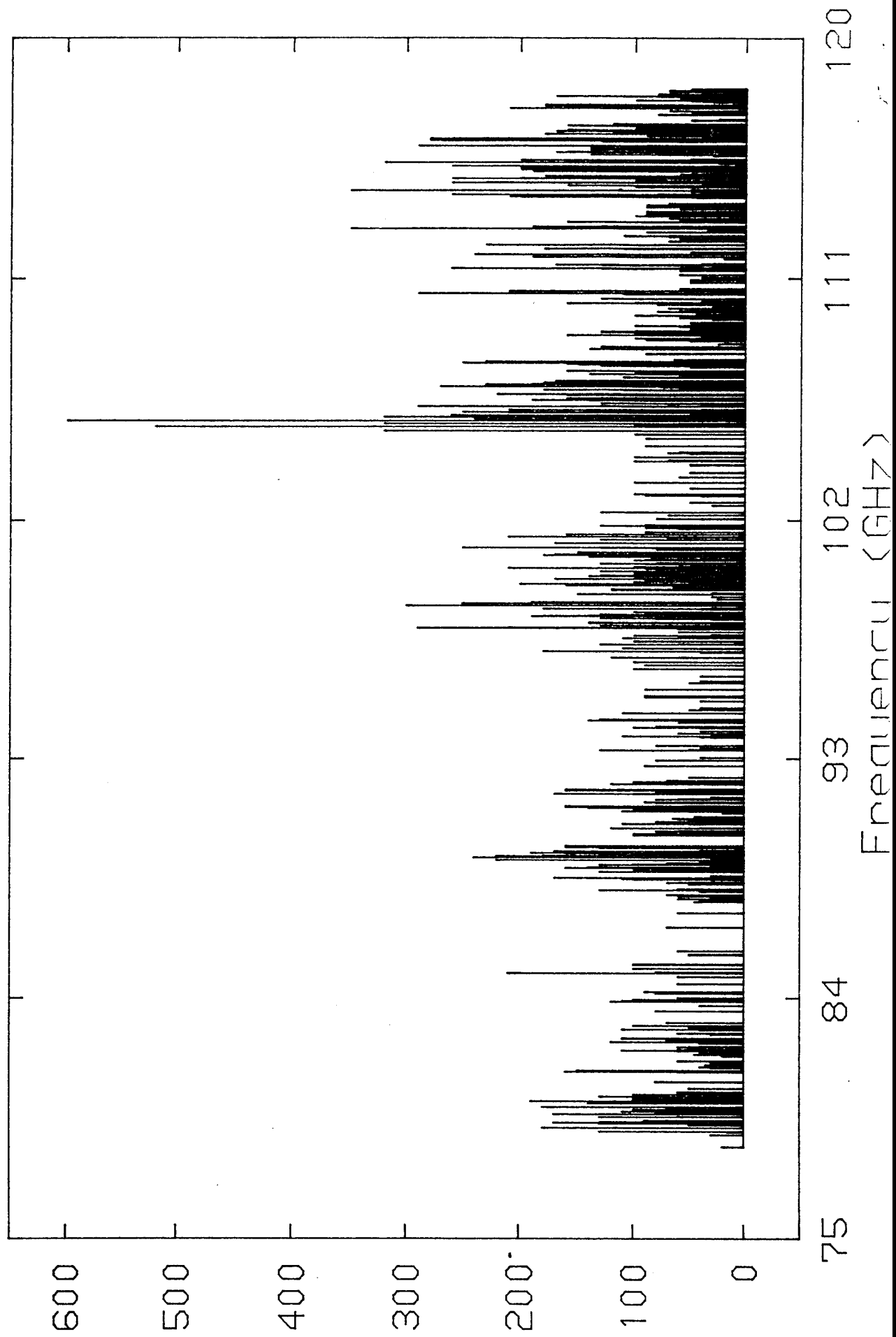




# Calculated



# Observed



# RDX Pyrolysis Products

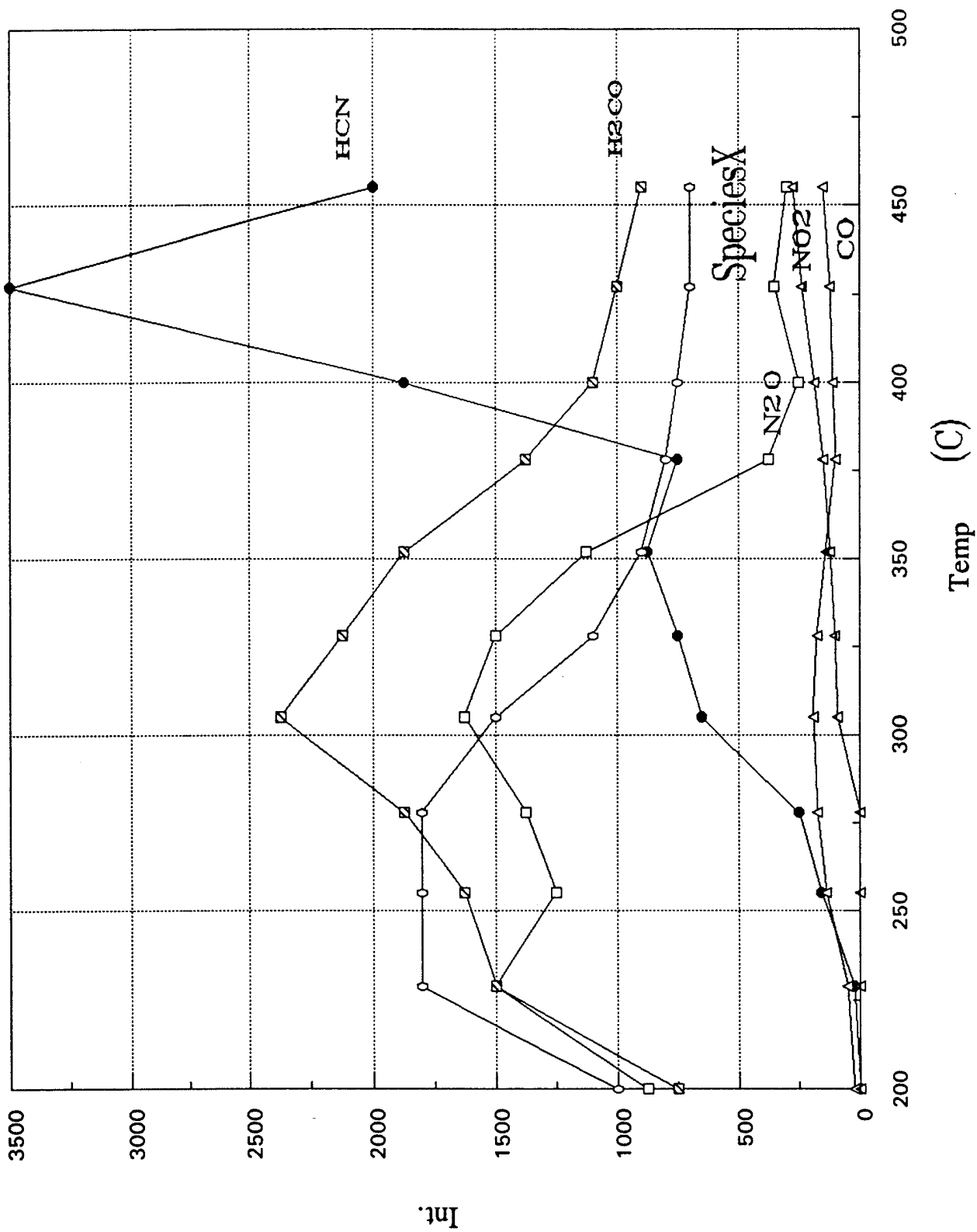


TABLE I. Microwave Transitions Identified in Heated Nozzle FTMW Study of RDX

Frequency	Species	Transition	Comments
14488.47	H <sub>2</sub> CO	2(1,1) - 2(1,2)	S/N = 30
25123.30	N <sub>2</sub> O	1 - 0	S/N = 40
23541.491	HONO	1(0,1) - 0(0,0)	S/N = 0.21
21982.097	HNCO	1(0,1) - 0(0,0)	S/N = 0.13
9237.027	NH <sub>2</sub> CHO	3(1,2) - 3(1,3)	S/N = 0.13
15392.501	NH <sub>2</sub> CHO	4(1,3) - 4(1,4)	S/N = 0.5
21207.234	NH <sub>2</sub> CHO	1(0,1) - 0(0,0)	S/N = 0.7

TABLE II. Microwave Transitions Identified in Pyrolysis MW Study of RDX

Frequency	Species	Transition
66973.496	H <sub>2</sub> CO	12(2,10)-12(2,11)
72409.097	H <sub>2</sub> CO	1(0,1) - 0(0,0)
72838.948	H <sub>2</sub> CO	5(1,4) - 5(1,5)
78230.50	H <sub>2</sub> CO	21(3,18)-21(3,19)
116718.615	H <sub>2</sub> CO	14(2,12)-14(2,13)
127154.96	H <sub>2</sub> CO	23(3,20)-23(3,21)
145389.34	H <sub>2</sub> CO	v <sub>5</sub>
145603.64	H <sub>2</sub> CO	2(02) - 1(01)
146635.3	H <sub>2</sub> <sup>13</sup> CO	2(02) - 1(01)
150400.72	H <sub>2</sub> CO	v <sub>5</sub>
75369.22	N <sub>2</sub> O	3 - 2
125613.92	N <sub>2</sub> O	5 - 4
125663.52	N <sub>2</sub> O	5 - 4
125901.28	N <sub>2</sub> O	5 - 4
125948.00	N <sub>2</sub> O	5 - 4
125948.96	N <sub>2</sub> O	5 - 4
53721.74	HCN	15 - 15
60861.65	HCN	16 - 16
68441.92	HCN	17 - 17
76461.46	HCN	18 - 18
84919.16	HCN	19 - 19
88630.416	HCN	1 - 0 F = 1 - 1
88631.847	HCN	1 - 0 F = 2 - 1
88633.936	HCN	1 - 0 F = 0 - 1
93813.84	HCN	20 - 20
103144.25	HCN	21 - 21
112909.10	HCN	22 - 22
65699.74	HNCO	3(1,3) - 2(1,2)
65946.17	HNCO	3(0,3) - 2(0,2)
65181.97	HNCO	3(1,2) - 2(1,1)
109498.34	HNCO	5(1,5) - 4(1,4)
109833.	HNCO	5(3 ) - 4(3 )
109875.8	HNCO	5(2 ) - 4(2 )
109908.95	HNCO	5(0,5) - 4(0,4)
109959.	HNCO	33(1,33) - 34(0,34)
113736.30	HNCO	43(0,43) - 42(1,42)
70588.6	NO <sub>2</sub>	7(1,1) - 8(0,8)
70646.2	NO <sub>2</sub>	7(1,1) - 8(0,8)
70654.1	NO <sub>2</sub>	7(1,1) - 8(0,8)
150439.22	NO	3/2,3/2-1/2,3/2

TABLE II. Microwave Transitions Identified in Pyrolysis MW Study of RDX  
(CONTINUED)

Frequency	Species	Transition
109753.59	NH <sub>2</sub> CHO	5(1,4) - 4(1,3)
127112.854	NH <sub>2</sub> CHO	6(2,5) - 5(2,4)
127330.361	NH <sub>2</sub> CHO	6(5 ) - 5(5 )
127348.704	NH <sub>2</sub> CHO	6(4 ) - 5(4 )
127393.783	NH <sub>2</sub> CHO	6(3,4) - 5(3,3)
127412.357	NH <sub>2</sub> CHO	6(3,3) - 5(3,2)
128102.967	NH <sub>2</sub> CHO	6(2,4) - 5(2,3)
148223.377	NH <sub>2</sub> CHO	7(2,6) - 6(2,5)
148556.391	NH <sub>2</sub> CHO	7(6 ) - 6(6 )
148567.324	NH <sub>2</sub> CHO	7(5 ) - 6(5 )
148599.5	NH <sub>2</sub> CHO	7(4 ) - 6(4 )
148667.617	NH <sub>2</sub> CHO	7(3,5) - 6(3,4)
148709.342	NH <sub>2</sub> CHO	7(3,4) - 6(3,3)
149792.812	NH <sub>2</sub> CHO	7(2,5) - 6(2,4)
98087.42	HONO	6(1,5) - 6(0,6)
104237.45	HONO	7(1,6) - 7(0,7)
111551.60	HONO	8(1,7) - 8(0,8)
113841.170	HONO	5(1,5) - 4(1,4)
117281.36	HONO	5(0,5) - 4(0,4)
115271.207	CO	1 - 0
112287.11	HCOOH	5(2,4) - 4(2,3)
112432.40	HCOOH	5(4) - 4(4)
112459.72	HCOOH	5(3,3) - 4(3,2)
112466.92	HCOOH	5(3,2) - 4(3,1)
112254.80	CH <sub>3</sub> CHO	6(1,6) - 5(1,5) E

TABLE III. Species Identified by Mass Spectrometry and Microwave Spectroscopy

	Mass Spectrometry <sup>1</sup>	This Work
H <sub>2</sub> O	yes	no line in range
HCN	yes	yes
CO	yes	yes
H <sub>2</sub> CO	yes	yes
NO	yes	yes
N <sub>2</sub> O	yes	yes
NO <sub>2</sub>	yes	yes
HNCO	NO	yes
HONO	yes	yes
NH <sub>2</sub> CHO	yes	yes
CH <sub>3</sub> NHCHO	yes	NO
oxy-s-triazine	yes	spectrum unknown
ONDNTA <sup>2</sup>	yes	spectrum unknown
HCOOH	NO	yes
CH <sub>3</sub> CHO	NO	yes?

1. Behrens & Bulusu, JPC **96**, 8877-8891 (1992).
2. 1-Nitroso-3,5-dinitrohexahydro-s-triazine

TABLE IV. Species X Rotational Parameters

Quantum Numbers	Observed Transitions		Rotational Parameters		
	Obs. Freq. <sup>a</sup>	Obs.-Calc. <sup>a</sup>	Constant	Value <sup>a</sup>	
2 <sub>12</sub> -1 <sub>11</sub>	70419.817	0.012	A (MHz)	141019.(58)	
2 <sub>02</sub> -1 <sub>01</sub>	72801.475	-0.002	B (MHz)	19417.002(13)	
2 <sub>11</sub> -1 <sub>10</sub>	75249.200	-0.003	C (MHz)	17002.124(12)	
3 <sub>13</sub> -2 <sub>12</sub>	105605.596	-0.170	$\Delta_{JK}$ (kHz)	645.3(44)	
3 <sub>03</sub> -2 <sub>02</sub>	109111.140	0.066	$\Delta_J$ (kHz)	36.43(43)	
3 <sub>22</sub> -2 <sub>21</sub>	109238.000	0.047	$\delta_J$ (kHz)	5.60(34)	
3 <sub>12</sub> -2 <sub>11</sub>	112848.900	0.038	$\Delta I$ (uÅ <sup>2</sup> )	0.113	
4 <sub>14</sub> -3 <sub>13</sub>	140763.310	-0.155			
4 <sub>04</sub> -3 <sub>03</sub>	145311.620	-0.023			
4 <sub>23</sub> -3 <sub>22</sub>	145618.800	-0.033			
4 <sub>13</sub> -3 <sub>12</sub>	150418.140	0.000			
5 <sub>15</sub> -4 <sub>14</sub>	175884.350	0.099			

a. In MHz

TABLE V. Candidate molecular sources for Species-X

CC	CN	CO	NN	NO	OO
HCCH	HCN	HCO	HNN	HNO	HOOH
CH <sub>2</sub> =CH <sub>2</sub>	CH <sub>2</sub> =NH	H <sub>2</sub> CO	H <sub>2</sub> NNH <sub>2</sub>	H <sub>2</sub> NOH	
CH <sub>3</sub> CH <sub>3</sub>	CH <sub>3</sub> NH <sub>2</sub>	CH <sub>3</sub> OH			
<b>Species</b>	<b>A (GHz)</b>	<b>B (GHz)</b>	<b>C (GHz)</b>		
<b>Species-X</b>	<b>141.0</b>	<b>19.42</b>	<b>17.00</b>		
CH <sub>2</sub> =NH	196.2	34.6	29.3		
CH <sub>3</sub> NH <sub>2</sub>	103.1	22.63	21.71		
H <sub>2</sub> CO	281.9	38.8	34.0		
CH <sub>3</sub> OH	127.6	24.69	23.78		
H <sub>2</sub> NNH <sub>2</sub>	143.4	24.08	24.07		
H <sub>2</sub> NOH	190.9	25.2	25.1		
HNCO	918.5	11.07	10.9		

# APPENDIX 1. Spectral Line Survey of RDX Decomposition Products

Frequency	Intensity ( $\mu\text{V}$ )						
53 721.630	300	very slow +		70 754.000	50		
53 852	30			70 760.600	50		
53 962	30			71 650.800	30		
54 062	30			71 669.220	70		
54 097	40			71 684.200	50		
54 207	30			72 801.740	260	slow + -	
54 310	40			75 249.190	900	very slow -	slow +
54 403	40	slow +		76 461.350	200	very slow +	
54 931	30			78 437	20		
59 342.340	40			78 876.930	30	+	
59 929	30			78 978	15		
59 947	30			79 004.820	130		
60 285	30	slow +		79 135.980	180		
60 612	50			79 232.700	30 \		
60 861.600	260	very slow +		79 234.460	50 /		
65 232	30	-		79 249.160	30		
65 653	70			79 298.420	130		
65 880	40	-		79 338.570	170		broad
66 083	30			79 363.260	130	+	
66 249	30			79 408.180	90		
67 033	30	-		79 411.980	70		
67 218	70	+		79 544.080	130		
67 275	30			79 560.760	60		
67 833	40			79 652.380	130		
67 893	60			79 656.420	170		
68 286	30			79 720.200	80		
68 441.800	230	very slow +		79 744	25	?	
68 634	50	slow +		79 751.250	110		broad
68 752	60	slow +		79 779.380	30		
68 908	30			79 789.560	100		broad
69 384	40			79 795.860	60	+	
69 411	50	slow -		79 835.840	100		
69 442	40			79 852.120	70		
69 555	50			79 885.700	30		
69 613	50			79 917.480	180		
69 628	40						
70 364.640	30			80 054.580	140		
70 385.600	40			80 116.540	130		
70 419.800	500	very slow -	slow +	80 140.800	190	-	
70 429.800	30			80 169.450	100		
70 603.300	30			80 181.980	80		
70 605.900	30			80 190.740	30	slow -	
70 620.700	40			80 208.620	60		
70 621.900	30			80 220.020	50		
70 640.660	40			80 235.040	100		
70 676.500	30			80 291.320	30	slow -	
70 706.100	30			80 302.880	50		
70 728.700	30			80 313.660	130		
70 731.900	50			80 385.080	100		
				80 405.500	60		broad

80 414.780	40				
80 420.160	60				
80 421.900	40		83 063	70	+
80 433.120	40		83 505.440	80	
80 477.620	60 \		83 701	40	
80 479.780	60 /		83 860.360	120	-
80 609	50	+	83 894.400	110	slow -
80 843.060	70		83 940.320	100	
80 860.780	80		83 995.680	60	
81 212.740	60				
81 241.560	160 \		84 168.475	80	-
81 242.760	120 /		84 205	60	
81 255.600	95		84 234.530	90	-
81 283.760	150	-	84 524.820	60	very slow +
81 368	30		84 788	60	-
81 415	40		84 919.120	210	very slow +
81 488	30		84 966	80	
81 491	35				
81 568	30		85 101	100	+
81 571	30		85 245.700	100	
81 627.220	60		85 265.660	100	
81 629.600	60		85 612	50	
81 807	20		85 637	50	
81 871.620	40		85 759	60	-
81 876.870	45				
81 901	20		86 655	70	
81 934.650	40				
81 941.900	20		87 197.830	60	+
81 946.430	30		87 619.670	45	
81 973	25		87 677.590	40	
			87 729	60	slow -
82 008.440	60		87 737	30	
82 029.540	110		87 757		
82 058.760	60		87 767		
82 075.900	50		87 821.900	60	slow +
82 145.180	60		87 886.850	70	broad
82 165.780	50				
82 182.240	40		88 003.200	40	
82 283	40		88 010.000	40	
82 298	40		88 066.710	130	
82 348	120		88 084.300	50	
82 402.420	40	slow -	88 101	60	
82 418.160	70		88 278	50	
82 470.360	110	slow -	88 337.600	70	
82 481.100	40	slow +	88 343.880	60	
82 487.980	110		88 349.800	50 \	
82 623.800	30		88 351.020	50 /	
82 670.160	60		88 444.740	30	slow -
82 681.100	50		88 462.020	100	
82 789	40	slow -	88 480.470	110	
82 821.500	110		88 520.210	170	
82 890.340	50	slow +	88 570.800	30	
82 946.560	40	-	88 586.200	30	
82 964.380	100		88 594.880	30	
			88 743.700	30	

88 748.750	130		90 252.300	50 /	
88 779.600	30	slow +	90 267.180	80	
88 794.400	70		90 285.160	60	+
88 801.560	100		90 368.740	120	
88 871.260	100		90 388.040	40	
88 877.600	80		90 528.360	50	
88 889.450	160		90 548.450	110	
88 895.460	130		90 567.900	30 \	
88 901.100	30		90 569.700	30 /	
88 914.660	30		90 584.400	30	slow +
88 921.080	140		90 614.700	30	
88 940.000	30		90 618.860	80	
88 960.800	30		90 670.780	30	
			90 680.700	50	
			90 710.670	60	
89 010.920	130		90 728.300	30	
89 034.360	100		90 741.920	65	slow ? +
89 079.260	70		90 747.900	40	
89 106.900	30		90 784.700	30	
89 114.000	30		90 813.020	45	
89 118.800	40		90 932	20	
89 143.420	40 \ ?				
89 144.050	40 / ?				
89 191.160	220		91 001.220	50	
89 211.800	30		91 015.100	30	
89 258.600	30		91 020.920	110	
89 279.620	240		91 027.360	110	
89 329.670	220		91 035.520	50	
89 359.880	180		91 075.440	80 \	
89 377.860	130		91 077.860	80	
89 388.660	110		91 079.560	50 /	
89 426.180	130		91 100.620	100	
89 438.780	160		91 105.360	40	slow +
89 443.760	30		91 115.180	50	
89 455.400	190		91 122.740	50	
89 474.700	30		91 143.220	140	
89 505.900	30		91 153.820	80	
89 515.620	170		91 172.760	160	
89 551.560	40	+ -	91 186.860	60 \	
89 634.840	130		91 191.200	70	
89 665.620	70		91 197.000	80 /	
89 670.660	160		91 208.160	160 \	
89 685.100	80		91 211.140	80 /	
89 717.980	160		91 216.740	50	
			91 316.720	80	
			91 329.760	50	
90 112.320	100 \		91 353.880	70	-
90 113.600	100		91 363.360	90	
90 114.580	90 /		91 446.620	80	
90 164.620	100		91 474.420	60	
90 183.400	50 \		91 481.660	50	
90 184.560	50 /		91 533.500	30	slow +
90 238.130	80		91 666.700	170	
90 246.520	50 \		91 669.360	50	
90 248.100	30		91 672.740	100	
90 250.500	40				

91 689.620	50		96 372	100	slow +
91 731.380	80		96 520	90	
91 760.320	70		96 635	100	
91 791.960	160		96 802	120	
91 831.200	160		96 807	60	
91 846.920	50		96 994	40	
92 029.000	30		97 042.240	180	
92 043.830	120	-	97 135.160	40	slow -
92 111.680	100		97 149.400	100	
92 120.100	100		97 158.780	110	
92 144.120	30	slow -	97 300.600	130	
92 155.960	30		97 319.840	60	
92 160.240	40	slow -	97 408.080	100	
92 175.440	70		97 427.540	100	
92 281.660	50		97 432.340	90	
92 719	90		97 539.400	110	
92 931	80		97 579.640	60	
92 943	60		97 640.800	100	
93 028	40		97 677.620	30	
93 305.040	130		97 777.500	60	
93 335.120	50	slow -	97 883.920	60 \	
93 401	40		97 885.240	50 /	
93 485.040	80		97 896.340	60	
93 796	30		97 906.500	40 \	
93 813.770	40	very slow +	97 907.980	40 /	
93 843.480	110	slow -	97 920.380	50	
93 909.580	30		97 928.920	50	
93 920.960	30		97 929.720	290 \	
93 926.860	30	slow-	97 934.200	290 }	very slow +
93 935.500	30		97 941.800	210 /	
93 952.800	60	slow +	98 001.620	110	
94 035	40		98 013.960	70	
94 144.800	40		98 023.620	130	
94 172.400	100	slow -	98 031.160	30	
94 210.600	80	slow -	98 086.840	30	slow +
94 354.580	60		98 107.520	140 \	
94 389.780	50		98 120.960	140 }	very slow +
94 435.460	140	slow -	98 134.800	140 /	
94 479.820	130	slow -	98 246.500	30	
94 706.040	110	+	98 275.600	80	
94 837	50		98 278.920	30 \	slow -
94 909	40		98 281.120	20	slow -
95 169	40		98 283.400	7 /	slow -
95 312	90	+	98 283.880	80	
95 362	90	slow -	98 293.120	130	
95 606	90	broad	98 346.600	30	
95 854	50	slow +	98 368.280	190	CH3CHO ?98 367.696
95 917	40	slow +	98 375.540	120	
96 107	40	broad	98 377.360	120	
			98 379.450	180	
			98 392.920	140	+
			98 399.800	90	

98 412.660	100	
98 437.920	130	
98 453.200	30	
98 454.840	90	
98 527.110	100	+
98 623.800	30	
98 635.900	40	slow +
98 651.140	180	
98 655.500	40	
98 671.500	30	\
98 673.300	30	
98 676.100	30	/
98 767.310	300	-
98 781.820	60	
98 789.200	30	
98 791.040	30	
98 823.500	30	
98 832.400	30	
98 841.400	30	
98 851.700	250	
98 854.080	50	
98 867.360	30	
98 882.200	30	
98 888.900	30	
98 897.720	190	
99 001.180	25	
99 093	30	
99 198.330	150	
99 248	30	
99 347.960	120	
99 383.550	120	
99 391.540	65	
99 406.500	50	
99 422.840	65	
99 460.840	30	
99 472.600	30	+
99 490.160	65	
99 524.840	160	
99 560.940	80	
99 573.640	50	\
99 575.320	110	/
99 583.510	200	
99 653.440	50	
99 660.160	50	
99 663.660	100	
99 711.480	40	
99 718.280	50	
99 728.800	90	
99 739.940	30	slow -
99 750.380	50	very slow -
99 765.360	90	
99 769.300	140	\
99 771.120	170	/

99 804.140	100	
99 825.220	40	
99 838.940	70	
99 877.780	140	\
99 881.120	130	/
99 902.640	130	
99 905.440	50	
99 924.820	50	\
99 926.020	70	/
99 955.100	100	+
99 965.040	90	\ -
99 968.480	60	
99 970.660	70	/
99 995.440	90	
100 002.800	40	
100 004.640	60	
100 011.220	40	
100 014.360	100	
100 027.780	60	+
100 053.320	60	\
100 054.780	45	
100 055.900	45	/
100 063.330	130	
100 070.660	80	
100 087.960	30	-
100 129.780	50	
100 133.290	60	
100 144.040	40	
100 146.160	90	
100 156.890	60	-
100 175.480	50	
100 184.330	210	
100 218.140	80	\
100 220.780	80	
100 224.560	50	/
100 234.620	100	
100 242.300	40	\
100 245.120	60	
100 247.840	50	/
100 324.860	90	
100 341.320	80	
100 351.200	130	\
100 353.000	60	/
100 363.400	80	\
100 366.620	60	/
100 384.380	80	
100 469.060	40	
100 474.620	100	
100 479.800	50	\
100 482.040	60	/
100 506.180	90	
100 517.520	60	
100 524.280	85	

CH3CHO 100 130.239

100 526.480	40		104 528.050	50	very slow +
100 610.560	140 \		104 557	70	
100 612.540	130 /		104 583	60	broad
100 616.820	100	slow -	104 590	40	slow +
100 638.760	60		104 814	90	slow +
100 646.440	100				
100 650.180	80		105 098	90	
100 674.260	180		105 246	90	
100 708.580	170		105 258	100	
100 759.380	90		105 354.100	40	-
100 775.920	60		105 385.900	320	
100 777.880	150		105 543.340	520	+
100 781.900	40		105 605.590	100	slow +
100 878.600	80		105 625.600	60	slow +
100 892.350	60		105 653.000	320	
100 901.050	40		105 665.030	40 \	
100 908.150	40		105 666.240	60 /	
100 922.750	40		105 754.830	600	- + 50 V
100 938.750	50 NH <sub>2</sub> CHO	100 922.291	105 773.680	200	
100 952.300	130		105 775.700	50	
100 960.880	250		105 800.600	50	
			105 810.060	30 \	
101 120.130	170		105 812.400	30 /	
101 258.160	130		105 817.560	50	
101 341	70		105 832.340	240	
101 375.660	210		105 877.420	50	
101 456.810	160		105 891.710	270	+
101 541	90		105 910.520	320	
101 678	60		105 946.800	100	slow +
101 711.010	90		105 957.600	40	
101 787.930	130		105 972.540	260	
101 820	90				
			106 023.160	50	slow -
102 052	40		106 067.480	210 \	
102 064.230	80 NH <sub>2</sub> CHO	102 064.3	106 069.490	210 /	
102 203	70	-	106 093.520	250	
102 308.070	130		106 096.180	50	
102 567.320	30	slow -	106 107.720	110	
102 682.620	50	slow +	106 134.780	60	
102 934.180	40	slow -	106 141.000	70	
102 958	90		106 146.200	140	
			106 151.860	100	
103 008.910	100		106 172.240	210	
103 223.400	50	slow +	106 183.860	40	
103 448.280	100	slow -	106 300.200	290	
103 642	60	slow -	106 307.180	130	
103 808	50		106 358.600	40	
103 821	50		106 396.820	70	
			106 409.500	130	
104 091	50		106 513.320	140	+
104 119	50		106 533.700	190	
104 237	100	+	106 541.580	140	
104 286	70		106 569.340	40	-
104 398	100		106 600.240	160	

106 606.300	130 \	
106 608.260	100 /	
106 715.330	160 \	
106 718.100	130 /	
106 751.820	220	
106 897.500	110	
106 914.420	180	
106 971.580	60	
107 013.820	45 CH3OH	107 013.85
107 017.780	75 + -	
107 023.790	50	
107 034.590	270 +	
107 036.840	25	
107 041.740	40	
107 044.620	40	
107 045.600	30	
107 057.110	160	
107 107.770	230	
107 123.320	190	
107 175.460	30	
107 178.960	30	
107 182.330	180	
107 195.370	130 +	
107 232.560	100	
107 243.680	170 \	
107 245.010	160 /	
107 364.620	40	
107 367.280	110	
107 372.860	30	
107 376.020	30	
107 377.090	110	
107 419.570	20 slow -	
107 448.280	60	
107 494.240	140	
107 499.420	80 \	
107 500.560	60 /	
107 559.510	100	
107 582.110	90 -	
107 619.800	160	
107 746.040	50	
107 797.340	130	
107 814.940	50	
107 845.700	150	
107 870.520	160	
107 904.630	250	
107 949.920	100	
107 956.490	230	
107 973.200	60	
107 989.320	40 slow +	
108 010.540	25	
108 014.780	15	
108 028.930	65	
108 238	90	

108 245.200	80 +	
108 408.810	140	
108 418.360	50	
108 454.520	60	
108 492.890	130	
108 589.740	25 \	
108 590.600	15 /	
108 609.210	20	
108 704	50	
108 740.720	90 +	
108 748.540	30	
108 797.380	100	
108 804.300	45	
108 809.760	25	
108 822.510	40	
108 857.940	40	
108 919.760	160	
108 937.100	30	
108 943.300	100 \	
108 944.690	100 /	
108 959.820	100 \	
108 960.360	100 /	
109 009.880	30 -	
109 019.890	60 +	
109 031.040	130 \	
109 031.740	130 /	
109 040.910	130	
109 048.640	130	
109 072.210	100	
109 105.870	40 \	
109 108.050	40 /	
109 115.140	50	
109 121.480	40	
109 126.610	20	
109 127.680	50	
109 138.720	35 CH3OH	109 138.71
109 149.850	40	
109 162.900	30 slow +	
109 187.050	50 \	
109 188.250	50 /	
109 194.900	40 slow -	
109 198.720	20	
109 209.450	50	
109 238.080	60 ?	
109 263.400	100	
109 269.950	50	
109 274.500	40	
109 278.240	40	
109 283.400	40 -	
109 361.800	50 slow -	
109 367.750	40	
109 372.250	30	
109 375.870	50 \	
109 377.050	40	

109 380.500	40 /		112 105.060	110 \ -	
109 482.560	30	slow +	112 105.560	110 /	
109 538.620	50		112 114.860	180 -	
109 547.350	40		112 254.800	230 CH3CHO	112 254.48 6(1,6) - 5(1,5) E
109 553.360	60	slow +	112 287.110	100 HCOOH	112 287.12 5(2,4) - 4(2,3)
109 556.690	35		112 382.950	70	
109 604.660	60	slow -	112 432.400	100 HCOOH	112 432.30 5(4,2) - 4(4,1)
109 640.050	100		112 459.720	100 HCOOH	112 459.60 5(3,3) - 4(3,2)
109 692.980	45		112 466.920	100 HCOOH	112 467.00 5(3,2) - 4(3,1)
109 776.480	60 \		112 469.240	60	
109 779.540	80 /		112 543.670	70 slow -	
109 785.340	50		112 545.610	40	
109 806.940	50 \		112 567.750	30 slow +	
109 807.900	60 /		112 586.360	110 \	
109 824.660	40		112 587.460	70 /	
109 890.880	50		112 714.980	90 slow +	
109 905.580	70	slow +	112 727.560	70	broad
109 956.140	30		112 775.500	35	
110 030.460	80		112 848.900	350 slow -	
110 089.140	160		112 860.800	30	
110 104.720	80		112 891.440	50 HCOOH	112 891.41 5(2,3) - 4(2,2)
110 110.920	100		112 896.080	80	
110 156.900	30		112 899.120	40	
110 164.240	40		112 926.390	70 slow -	
110 254.920	130		112 938.370	190 \slow -	
110 418.960	110		112 941.850	130 /slow -	
110 460.980	290		113 083	30 -	
110 523.580	30		113 108.920	160	
110 548.540	210		113 111.720	160 slow -	
110 619	60 -		113 157	60	
110 855	50		113 162	50	
110 948	50	slow +	113 232.000	70	
111 028.770	40		113 321.979	90	
111 047.550	40	broad	113 323.530	100	
111 133	60		113 379.100	90	
111 285	60		113 430.130	90 slow +	
111 319.480	40		113 492.410	90	
111 328.940	40		113 580	60 slow -	
111 336.240	40		113 660	90 slow +	
111 365.860	40		113 705	40 slow +	
111 367.860	130		113 736	90 slow +	
111 384.070	260 -		113 786	70	
111 402.420	60	slow -	113 841.170	45 slow +	HONO 113 841.03 5(1,5) - 4(1,4)
111 474.420	30	slow +	114 003.820	20 \slow +	
111 497.480	130		114 005.340	45 slow +	
111 514.590	170		114 006.940	7 /slow +	
111 540.660	40	slow +	114 019.200	30	
111 551.150	30	slow + ?	114 034.000	50	
111 723	20		114 043.160	200	
111 806.290	190 -		114 058.590	210	
111 899.300	240 -		114 069.080	30	
111 917.140	30	slow -	114 123.790	260	
111 923.860	40	slow +	114 134.940	50	
111 982.190	50	very slow -	114 141.220	30	

114 148.700	80 \	
114 149.640	40 /	
114 166.400	40	
114 233.020	50 -	
114 278.150	350	
114 312	50	broad
114 408.960	100	broad
114 471.280	160	slow -
114 534.600	40	broad
114 576.380	260	
114 582.860	70	broad
114 589.500	30	
114 598.240	230	
114 602.520	70	
114 643.920	30	
114 650.880	30	
114 662.700	100	
114 727.400	260	
114 736.370	150	
114 748.000	200 \	
114 749.160	200 /	
114 750.560	40	CH3OH 114 750.70
114 764.940	40	
114 786.980	170	
114 803.120	110	
114 806.620	30	
114 816.020	80 \	
114 818.700	50	
114 832.840	30	
114 843.350	180	
114 890.300	30	
114 893.780	40	slow +
114 903.770	60	slow -
114 906.900	50	
114 975.580	30	
114 996.290	190	
115 019.130	160	
115 036.920	70	
115 061.660	90	
115 063.170	20	
115 070.780	200	
115 106.330	65	
115 110.810	200	
115 119.750	200	
115 144.120	65	
115 146.740	200	slow -
115 155.180	200	
115 203.850	260	
115 291.540	20	\slow +
115 293.540	25	slow +
115 295.520	15	/slow +
115 338.220	160 \	
115 339.960	320 /	
115 410.120	100	

115 426.300	60	
115 434.570	200	
115 462.540	50	
115 563.040	30	
115 628.420	140	
115 634.620	80	slow +
115 710.560	15	\slow +
115 711.640	15	slow +
115 712.720	15	/slow +
115 716.520	170	
115 725.860	140	C2H5CN-? 115 725.965
115 734.210	160	
115 804.740	90	slow +
115 810.300	30	
115 815.880	140	
115 843.800	40	
115 846.760	110	
115 856.400	100	
115 881.500	140	
115 892.060	60	
115 902.440	50	
115 924.960	80	
115 934.860	65	
115 938.380	50	
115 960.220	290 \	
115 962.900	140 /	
115 971.180	90	
116 119.600	130	
116 161.390	270	
116 173.010	100	
116 176.870	280 \	
116 178.020	250 /	
116 235.590	280	
116 238.160	260	
116 241.340	260	
116 309.500	40	
116 340.050	90	
116 345.750	30	
116 378.050	30	
116 388.100	30	
116 412.080	180	
116 447.470	120	
116 514.050	170	
116 565.170	160	
116 618.320	100 \	
116 619.610	90 /	
116 646.720	20 \	
116 647.570	100 /	
116 711.440	15	CH3CHO 116 711.450
116 715.270	150	
116 725.650	160	
116 757	60	+
116 786.080	120	
116 922.500	50	

116 953.750	25		124 948	80	
117 137.360	50				
117 143.060	80		125 035.520	80	
117 149.600	60		125 062.940	120	
117 225.700	50		125 215	80	
117 281.700	70	slow -	125 318	100	
117 383.050	210		125 538	80	2 lines
117 436.770	90		125 684	100	
117 467.710	180		125 819	70	
117 514.420	180		125 887	80	
117 602.290	25				
117 605.600	30		127 553	80	
117 615.300	30				
117 626.600	30		131 155	50	
117 630.200	40		131 353	60	
117 641.000	30		131 508	90	+
117 651.940	50		131 618	40	slow +
117 678.420	100		131 628	70	
117 738.700	50		131 751	60	
117 741.200	60		131 813	90	
117 760.200	60	+ -	131 920	70	
117 766.360	50				
117 769.880	30		133 545	90	
117 777.000	30		133 556	100	broad
117 816.520	80		133 644	100	broad
117 831.890	170		133 712	60	-
117 842.380	80		133 722	80	
117 847.220	80	slow +			
117 870.980	80		134 105.020	80	
117 903.000	80		134 131.260	110	
117 911.760	40		134 139.980	190 \	
118 003.280	70		134 142.300	200 /	
118 006.420	70		134 165.700	80	slow -
118 026.610	50		134 201.880	200 \	
118 039.100	70		134 204.300	250 /	
118 070.770	40		134 256.220	100	
118 078.310	50		134 280.220	150	
118 086.470	50		134 348		100
118 092.200	7	CH3CHO 118 092.403	134 409.800	80 \	
118 093.840	40		134 414.600	80 /	broad
118 098.440	50 \		134 436.000	200	slow +
118 099.640	50	/HCOOCH3 118099.557	134 468.800	100	
123 508	40		134 481.520	450	very slow HNCO
123 648	40		134 565	80	
123 789	90	broad	134 606.400	70	slow -
			134 642.320	90	
124 085	80		134 676.080	90	
124 253	80		134 713.120	70	broad
124 306	80		134 720.420	80	
124 424	80		134 784.100	140	
124 455	80		134 788.880	160	
124 511	90		134 815.900	50	
124 905	90		134 830.000	130	
124 927	80		134 842.340	260	

134 870.980	200		143 519	60 /	
134 968.640	220 \	-	143 577	100	
134 971.620	100 /		143 582	100	
134 980.440	200		143 589	90	
135 101	150		144 133	90	
135 356	200		144 272	70	
135 394	150		144 439	60	
135 443	100		144 483	60	
135 597	150		144 681	70	
135 612.100	80	broad	144 827.920	150 \	slow ?
135 618.300	80		144 833.900	80 /	slow ?
135 648.440	100		144 906	100	
135 682.440	130				
135 705	60		145 116	100	
135 738	60		145 225	150	
135 772	90		145 370.000	70	
135 895	60		145 389.700	250	H2CO nu5
			145 450.600	80	
136 210	90		145 459.740	80	
136 234	80		145 477.300	130	
136 466	60		145 481.240	130	very slow +
136 497	60		145 505.420	60	
136 550	50	+	145 519.660	60	
136 594	60		145 535.220	90	
136 644	80		145 551.180	80	
			145 563.900	180	
140 721.180	60		145 574.180	200	
140 735.000	70		145 618.930	150	
140 752.800	150		145 650.260	500	slow +
140 763.310	1300		145 664.400	150	
140 808	130		145 681.300	80	
			145 685.820	80	
142 015	70		145 703.780	60	
142 030	70		145 710	90	
142 112	60		145 715	90	
142 129	60		145 732.500	80	
142 228	80		145 749.140	80	
142 414	80		145 762.300	90	
142 502	70		145 766.180	100	
142 511	130		145 769.900	90	
142 736	60		145 789.900	100	
142 740	60		145 792.520	150	
142 746	60		145 811.400	70	
142 838	70		145 819.520	80	
142 845	80		145 826.600	100	
142 860	80		145 836.400	100	
142 883	90		145 839.840	400	very slow +
142 896	70		145 910.500	40	+
			145 937.000	60	
143 108	60		145 943.400	100 \	
143 436	80		145 946.220	100	
143 454	80		145 947.540	100 /	
143 517	60 \		145 962.940	100	

145 971.220	30	-	149 820	100	
145 973.900	30		149 928	150	-
145 983.200	60				
145 988.540	60		150 021	150	
			150 094	190	
146 145.200	100	slow +	150 129.820	130	-
146 167.400	50		150 141.600	40	
146 175.640	60		150 150.000	300	
146 186.000	50		150 156.960	400	
146 507	70		150 206.800	70	
146 581	60		150 235.200	70	
146 686	60		150 268.720	70	
146 679	70		150 280.020	100	
146 673	50		150 297.080	240	
146 734	90		150 320.700	50	
146 837	80		150 330.000	60	
146 855	80		150 341.120	300	
146 862	80		150 383.840	100	
146 981	70	slow +	150 418.125	600	
			150 522.380	180	
147 209	60		150 562.240	100	
147 239	60		150 575.040	200	
147 329	130		150 600.620	150 \	
147 476	100		150 602.180	150 /	
147 566	90		150 626.340	200	
147 590	70		150 787.400	60	slow -
147 596	70		150 793.860	150	
147 618	100		150 794.820	110	very slow +
147 691	80		150 998	150	
147 761	200				
147 879.740	200	-	175 884.325	120	slow
148 069	90				
148 157	80				
148 347	80				
148 350	80				
148 544	70				
148 578	80				
148 598	70				
148 667	60				
148 696	70				
148 783	60				
148 993	150				
149 031	70				
149 086	70				
149 137	70	+			
149 163	60	+			
149 225	100				
149 234	100				
149 342	60				
149 381	100				
149 409	100				
149 607	70				