

H A R V A R D U N I V E R S I T Y

Department of Chemistry
12 Oxford Street
Cambridge 38, Massachusetts

May 1, 1964

Dear Contributor:

This is the seventh microwave spectroscopy information letter and is being sent to those who contributed.

1. UNIVERSITY OF BIRMINGHAM
Department of Chemistry
(John Sheridan)

CH_2FI	Fluoro-iodomethane	P. Curnuck	Assigned
$\text{C}_4\text{H}_3\text{OD}$ ($\text{CH}_3\text{CO}\cdot\text{CCD}$)		O. L. Stiefvater	Assigned
$\text{C}_4\text{H}_4\text{O}^{18}$ ($\text{CH}_3\text{CO}^{18}\cdot\text{CCH}$)		O. L. Stiefvater	Assigned
$\text{C}_3\text{H}_3\text{NO}$	Isoxazole	W. C. Mackrodt	Tentative Assignment

2. UNIVERSITY OF CALIFORNIA
Department of Chemistry
W. D. Gwinn
R. J. Myers

CH_3SF_5	Methyl Sulfurpenta- fluoride		Paper in progress
IF_5	Iodine Pentafluoride		Work in progress
CH_6OSi	Silyl methyl ether		Work in progress
$\text{C}_2\text{H}_5\text{N}$	Ethyleneimine		Quadrupole and barrier paper in progress
$\text{C}_3\text{H}_6\text{S}$	Trimethylene sulfide		Assignment, including excited states
C_4H_6	Cyclobutene		Paper in Progress
CF_3NO_2	Trifluoronitromethane		Paper in progress
CH_3NO_2 (CH_3ONO)	Methyl nitrite		Paper in progress
$\text{C}_4\text{H}_8\text{O}$	Tetrahydrofuran		Assignment, including excited states
$\text{C}_4\text{H}_7\text{Cl}$	Chlorocyclobutane		Paper in progress

(continued UNIVERSITY OF CALIFORNIA)

C_4H_6O	Dihydrofuran	Paper in progress
C_5H_8O	Cyclopentanone	Assignment, including excited states
C_2H_4ClN	Chloroaziridine	Assignment, including quadrupole splittings
C_4H_7F	Cyclobutyl fluoride	Paper in progress

3. COLUMBIA UNIVERSITY
Radiation Laboratory
(P. Cahill and P. Gold)

C_3OH_6	Methyl vinyl ether	Work in progress
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4. UNIVERSITY OF COPENHAGEN
Department of Chemical Physics
(Børge Bak)

C_3H_3NS	Thiazole	D(2), D(5) and ^{15}N -species assigned. Quadrupole of main species partly assigned.
C_3H_4O	Methyl Ketene	Three mono- ^{13}C -species and one deuterated species assigned.
C_4H_5N	Pyrrole	Main species reinvestigated at lower frequencies, dipole and quadrupole moment measured. ^{15}N , $^{13}C(2)$, and $^{13}C(3)$ -species assigned.
$C_6H_4F_2$	Ortho Difluorobenzene	Several Lines observed.

5. University of Freiburg
Physikalisches Institut, Universität Freiburg i.Br.
(W. Maier)

C_2H_6OS $((CH_3)_2SO)$	Dimethylsulfoxide	H. Dreizler U. G. Dendl	Normal, d-6, manuscript being prepared. C^{13}, S^{34}, O^{18} , centrifugal distortion in progress
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(continued UNIVERSITY OF FREIBURG)

C_3H_6O ($(CH_3)_2CO$)	Acetone	R. Peter	Normal, O ¹⁸ work on barriers in progress
		F. Mönnig	d-6, work completed
$C_3H_{12}NB$ ($(CH_3)_3N-BH_3$)	Trimethylamine-borane complex	H. G. Schirdewahn	Manuscript being prepared
C_7H_7F ($C_6H_4CH_3F$)	p-fluorotoluene	H.D.Rudolph	Just started.
C_2N_2S ($S(CN)_2$)	Sulfurdicyanide	H. Arnold U. G. Dendl	Assignment in progress

6. GEORGIA INSTITUTE OF TECHNOLOGY
School of Physics
(Quitman Williams and T. L. Weatherly)

$CFCl_3$	Trichlorofluoromethane	A. Wolf	Work continuing on quadrupole interactions
$CHCl_3$	Chloroform	A. Wolf	Work continuing on quadrupole interactions
SCl_2	Sulfur Dichloride	J. Murray	Assigned

7. HARVARD UNIVERSITY
Department of Chemistry
(E. B. Wilson, Jr.)

F_2S_2 (S_2F_2)	Sulfur monofluoride	R. Kuczkowski	Full paper in press.
F_4Oxe ($XeOF_4$)	Xenon oxyfluoride	J. Martins	Structure completed.
CH_3ClO (CH_3OCl)	Methyl hypochlorite	J. Rigden	In press.
C_2HF_3O (CF_3CHO)	Trifluoroacetaldehyde	C. Woods	Structure and barrier completed.
$C_2H_2N_2O$ ($H-C-N-O-N-CH$)	1,2,5-oxadiazole	E. Saegbarth	Manuscript in preparation
GeH_6Si (SiH_3GeH_3)	Silyl germane	R. Varma and P. Cox	Analyzed

(continued HARVARD UNIVERSITY)

FH_5Si_2 ($\text{SiH}_3\text{SiH}_2\text{F}$)	Disilanyl fluoride	P. Cox and R. Varma	Analyzed
HNO_3	Nitric acid (isotopes)	J. Riveros and P. Cox	Structure
$\text{C}_4\text{H}_8\text{O}$ ($\text{CH}_3\text{CH}=\text{CHCH}_3$)	trans 2-3 epoxy- butane	M. Emptage	Analyzed
$\text{C}_2\text{H}_2\text{F}_2\text{O}$ (CH_2FCFO)	fluoroacetyl fluoride	E. Saegbarth	One form analyzed
C_3OH_6	Methyl vinyl ether	N. Owen	Work in progress

✓ 8. UNIVERSITY OF JODHPUR
Physics Department
(G. P. Srivastava)

Jodhpur, India

$\text{C}_2\text{H}_3\text{FO}_2$ (CH_2FCOOH)	Monofluoroacetic acid	G. P. Srivastava	
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9. UNIVERSITÄT KIEL
Lehrstuhl für Chemische Physik
(Werner Zeil)

$(\text{CH}_3)_3\text{SiCCH}$	Trimethylaethinyl- silan	H. K. Bodenseh	Work in progress
$(\text{CH}_3)_3\text{SiCCD}$		R. Gegenheimer	

10. UNIVERSITY OF LOUVAIN
Institut de Physique Moléculaire
(M. de Hemptinne)

$\text{C}_2\text{H}_6\text{O}$ ($\text{C}_2\text{H}_5\text{-OH}$)	Ethyl alcohol	J. Michielsen- Effinger	Spectrum of the normal species and 5 isotopic species observed from 12 to 43 kMc. Manu- script prepared
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(continued UNIVERSITY OF LOUVAIN)

$C_2H_2F_2$ ($CH_2 = CF_2$)	Vinylidene fluoride	J.C. Chauffoureaux	Rotational constants of four excited states calculated. Manuscript prepared.
C_2H_3Br ($CH_2 = CHBr$)	Vinyl bromide	R.P. Savariraj	Transitions 3 → 4 assigned. Rotational constants of the first excited state calculated.
$S^{32}O^{16}O^{18}$	Oxygen sulfide	A. Defossez	Spectrum actually measured between 9.000 Mc and 40.000 Mc
$S^{36}O^{16}O^{16}$	Oxygen sulfide	R. Van Riet	Rotational constants calculated; manuscript prepared.

11. MICHIGAN STATE UNIVERSITY
Department of Chemistry
(R. H. Schwendeman)

$^{13}CD_3Cl$	Methyl chloride	J. Kelly	Manuscript in preparation
$^{13}CD_3Br$	Methyl bromide	J. Kelly	Manuscript in preparation
C_3H_7Br ($CH_3CHBrCH_3$)	2-Bromopropane	F. Tobiasson	Parent and C-13 species assigned
$C_4H_{10}Br$ ($(CH_3)_3CBr$)	t-Butyl bromide	D. Silverman	C-13 species assigned
C_2H_5NO ($CH_3CH:NOH$)	Acetoxime	R. Rogowski	One species of parent assigned
$C_2H_5BO_2$ ($CH_2OBHOCH_2$)	1,3,2-Dioxaborolane	J. Hand	Parent assigned
C_3H_7NO ($(CH_3)_2NCHO$)	Dimethylformamide	R. Schwendeman	Parent partially assigned.

12. NATIONAL BUREAU OF STANDARDS
Infrared and Microwave Spectroscopy Section
(David R. Lide)

SO radical		Powell and Lide	Manuscript in preparation
AlCl	Aluminum monochloride	Lide	Spectrum assigned
SO ₂ F ₂ (excited states)	Sulfuryl fluoride	Lide	Manuscript prepared
/ ClCN (excited states)	Cyanogen chloride	Lafferty and Lide	In progress
/ HBF ₂	Difluoroborine	Kasuya and Lide	Spectrum assigned
/ CH ₃ CCSiH ₃	Methylsilyl-acetylene	Kirchhoff and Lide	Almost complete
/ HNSO	Thionylimine	Kirchhoff	Spectrum assigned
? CH ₃ CH:CHCH ₃	<u>cis</u> -2-butene	Sarachman	Manuscript in Preparation
X HCOOH (excited states)	Formic acid	Sarachman	Abandoned
✓ ClO ₃ F	Perchloryl fluoride	Lide	Spectrum assigned

13. NATIONAL RESEARCH COUNCIL (OTTAWA)
Division of Pure Physics
(C. C. Costain)

C ₃ H ₄ O	Trans propenal (acrolein)	C.C. Costain	3 C ¹³ , O ¹⁸ and 6 D species assigned in manuscript
C ₅ H ₈	Cyclopentene	S.S. Butcher	Rotation-vibration interactions, in manuscript

14. UNIVERSITY OF OKLAHOMA
Department of physics
(C. C. Lin)

CH ₃ SCN		Kojima, Lin, Nakagaiva	Barrier determined
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15. UNIVERSITY OF PADUA
Institute of Physical Chemistry
(Paolo G. Favero)

NOCl		A. M. Mirri	Search for B-type transitions in the 2 to 1 mm region temporarily abandoned.
NOCl		P. G. Favero	Nitrogen quadrupole coupling: manuscript prepared.
NOBr		A. Guarnieri	Nitrogen quadrupole coupling
PCl ₃		A. M. Mirri	Millimetre wave spectrum for centrifugal analysis.
AsCl ₃			
NOBr			

16. QUEEN'S UNIVERSITY, ONTARIO
Physics Department
(David B. McLay)

Canada

CHFC1 ₂	Dichlorofluoro-methane	D. B. McLay	Paper to appear in Can. J. Phys.
CDCl ₃	Chloroform-d	D. B. McLay	Microwave spectra of asymmetric isotopic species

17. RICE UNIVERSITY
Department of Chemistry
(Robert Curl)

CH ₃ NOS (CH ₃ NSO)	Methyl N-Thionylamine	V. Rao	a-type assignment and barrier
C ₂ H ₅ N (CH ₃ N: CH ₂)	N-Methyl Methyl-enimine	K.V.L.N.Sastry	Accepted for publication.
C ₃ H ₄ O ₂ (CH ₂ :CHOOCH)	Vinyl formate	V. M. Rao	Accepted for publication

(continued RICE UNIVERSITY)

NO_2	Nitrogendioxide	J.A. Hodgeson	Proof returned.
$\text{N}^{14}\text{O}^{16}\text{O}^{17}$	O^{17} Nitrogen-dioxide	J.A. Hodgeson	Lines observed, computer programming completed.

18. STANFORD UNIVERSITY
Chemistry Department
(Victor W. Laurie)

$\text{C}_3\text{H}_9\text{N}$ $(\text{CH}_3)_3\text{N}$	Trimethylamine	J. Wollrab	Manuscript
$\text{C}_2\text{H}_7\text{N}$ $(\text{CH}_3)_2\text{NH}$	Dimethylamine	J. Wollrab	Manuscript
C_5H_8	Methyl cyclobutane	L. Scharpen	Several states assigned.
$\text{C}_4\text{H}_6\text{O}$	Cyclobutanone	L. Scharpen	Manuscript

19. UNIVERSITY OF STOCKHOLM
Institute of Physics
(H. Selen)

$\text{C}_6\text{H}_4\text{ClF}$	1-chloro- 2-fluorobenzene	P. Kokeritz	Manuscript in preparation
$\text{C}_6\text{H}_5\text{FO}$ $(\text{F}\cdot\text{C}_6\text{H}_4\cdot\text{OH})$	O-fluorophenol m-fluorophenol	H. Selen	Work in progress

20. SWISS FEDERAL INSTITUTE OF TECHNOLOGY
Physical Chemistry Department
(Hs.H. Gunthard)

$\text{C}_2\text{H}_3\text{NO}_2$ $(\text{CH}_2=\text{CHNO}_2)$	Nitroethylene	H. D. Hess	Manuscript prepared
$\text{C}_3\text{H}_5\text{Cl}$ $(\text{CH}_2=\text{CCl}-\text{CH}_3)$	Chloropropene	W. Good	Tentative assignments made

21. UNIVERSITY OF TEXAS
Department of Chemistry
(James E. Boggs)

C_2HF_3 ($CF_2:CHF$)	Trifluoroethylene	K. Dorris	Normal species completed.
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22. THE UNIVERSITY OF TOKYO
Department of Chemistry
(Yonezo Morino)

CH_2O , CD_2O (H_2CO , D_2CO)	Formaldehyde	K. Takagi T. Oka	Excited vibrational states, manuscript prepared
SO_2	Sulfur dioxide	Y. Kikuchi S. Saito E. Hirota	Excited vibrational states, equilibrium structure in press.
COS , $COSe$	Carbonyl sulfide Carbonyl selenide	C. Matsumura	Excited vibrational states, equilibrium structure work completed.
OF_2	Oxygen difluoride	S. Saito	Excited vibrational states, spectra in v_2 , v_3 states assigned
CF_2O (F_2CO)	Carbonyl fluoride	S. Saito	Excited vibrational states, manuscript prepared.
$ClNO_2$	Nitryl chloride	T. Tanaka	Excited vibrational states, manuscript prepared
FNO_2	Nitryl fluoride	T. Tanaka	Excited vibrational states, spectra partially assigned
CH_3Br	Methyl bromide	C. Hirose	Excited vibrational states, spectra in v_4 , v_5 , v_6 , $2v_3$ states assigned.

(continued THE UNIVERSITY OF TOKYO)

C_3H_5F ($CH_2=CHCH_2F$)	Allyl fluoride	E. Hirota	Rotational isomerism manuscript prepared
C_3H_5Cl ($CH_2=CHCH_2Cl$)	Allyl chloride	E. Hirota	Rotational isomerism gauche and cis forms detected, analysis in progress

23. UNIVERSITY COLLEGE
Chemistry Department
(D. J. Millen)

NOF	Nitrosyl fluoride	K. S. Buckton	Centrifugal distortion analysis made of $^{15}N^{16}OF$, $^{14}N^{18}OF$ and $^{14}N^{16}OF$
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↓ 24. STATE UNIVERSITY OF UTRECHT
Physical Laboratory
(H. A. Dijkerman)

*Utrecht
Netherlands*

$DCCOCH_3$	1-Methoxy ethyn-2D	D. den Engelsen	Spectrum assigned
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25. University of Wisconsin
Department of Chemistry
(C. D. Cornwell)

CH_3F_2P (CH_3PF_2)	Methyl difluoro phosphine	E. A. Cohen	Discontinued
CH_3F_4P (CH_3PF_4)	Monomethyl tetra- fluoro phosphorane	E. A. Cohen	In progress
F_5IO (IOF_5)	Iodine oxide penta- fluoride	S. B. Pierce	In progress

FORMULA INDEX

(Arrangement as in Townes and Schawlow.
Numbers refer to Institution)

$AlCl_3$	(aluminum monochloride) - 12	C_2HF_3	(trifluoroethylene) - 21
sCl_3	- 15	C_2HF_3O	(trifluoroacetaldehyde) - 7
rNO	- 15	$C_2H_2F_2$	(vinylidene fluoride) - 10
BrD_3	(methyl bromide) - 11	$C_2H_2F_2O$	(fluoroacetyl fluoride) - 7
ClD_3	(methyl chloride) - 11	$C_2H_2N_2O$	(1,2,5,-oxadiazole) - 7
ClN	(cyanogen chloride) - 12	C_2H_3Br	(vinyl bromide) - 10
Cl_3D	(chloroform-d) - 16	$C_2H_3FO_2$	(monofluoroacetic) - 8
Cl_3F	(trichlorofluoromethane) - 6	$C_2H_3NO_2$	(nitroethylene) - 20
F_2O	(carbonyl fluoride) - 22	C_2H_3SN	- 14
F_3NO_2	(trifluoronitromethane) - 2	C_2H_4ClN	(chloroaziridine) - 2
HCl_2F	(dichlorofluoromethane) - 16	$C_2H_5BO_2$	(1,3,2-dioxaborolane) - 11
HCl_3	(chloroform) - 6	C_2H_5N	(n-methyl methylenimine) - 17
H_2FI	(fluoro-iodomethane) - 1	C_2H_5N	(ethyleneimine) - 2
H_2O	(formaldehyde) - 22	C_2H_5NO	(acetoxime) - 11
H_2O_2	(formic acid) - 12	C_2H_6O	(ethyl alcohol) - 10
H_3Br	(methyl bromide) - 22	C_2H_6OS	(dimethylsulfoxide) - 5
H_3ClO	(methyl hypochlorite) - 7	C_2H_7N	(dimethylamine) - 18
H_3F_2P	(methyl difluoro phosphine) - 25	C_2N_2S	(sulfurdicyanide) - 5
H_3F_4P	(monomethyl tetrafluoro phosphorane) - 25	C_3H_3NO	(isoxazole) - 1
H_3F_5S	(methyl sulfurpentafluoride) - 2	C_3H_3NS	(thiazole) - 4
H_3NOS	(methyl n-thionylamine) - 17	C_3H_3DO	(1-methoxy ethyn-2D) - 24
H_3NO_2	(methyl nitrite) - 2	C_3H_4O	(trans propenal) - 13
H_6OSi	(silyl methyl ether) - 2	C_3H_4O	(methyl ketene) - 4
OS	(carbonyl sulfide) - 22	$C_3H_4O_2$	(vinyl formate) - 17
OSe	(carbonyl selenide) - 22		

(continued FORMULA INDEX)

C_3H_5Cl	(chloropropene) - 20	C_5H_8	(methyl cyclobutane) - 18
C_3H_5Cl	(allyl chloride) - 22	C_5H_8O	(cyclopentanone) - 2
C_3H_5F	(allyl fluoride) - 22	C_5H_9DSi	- 9
C_3H_6O	(acetone) - 5	$C_5H_{10}Si$	(trimethylaethynylsilan) - 9
C_3H_6O	(methyl vinyl ether) - 3,7	C_6H_4ClF	(1-chloro-2-fluorobenzene) - 19
C_3H_6S	(trimethylene sulfide) - 2	$C_6H_4F_2$	(ortho difluorobenzene) - 4
C_3H_6Si	(methylsilylacetylene) - 12	C_6H_5FO	(o-fluorophenol - 19 m-fluorophenol)
C_3H_7Br	(2-bromopropane) - 11	C_7H_7F	(p-fluorotoluene) - 5
C_3H_7NO	(dimethylformamide) - 11	$ClFO_3$	(perchloryl fluoride) - 12
C_3H_9N	(trimethylamine) - 18	$ClNO$	- 15
$C_3H_{12}NB$	(trimethylamineborane - 5 complex)	$ClNO_2$	(nitryl chloride) - 22
C_4H_3OD	- 1	Cl_2S	(sulfur dichloride) - 6
$C_4H_4O^{18}$	- 1	Cl_3P	- 15
C_4H_5N	(pyrrole) - 4	FH_5Si_2	(disilanyl fluoride) - 7
C_4H_6	(cyclobutene) - 2	FNO	(nitrosyl fluoride) - 23
C_4H_6O	(cyclobutanone) - 18	FNO_2	(nitryl fluoride) - 22
C_4H_6O	(dihydrofuran) - 2	F_2O	(oxygen difluoride) - 22
C_4H_7Cl	(chlorocyclobutane) - 2	F_2O_2S	(sulfuryl fluoride) - 12
C_4H_7F	(cyclobutyl fluoride) - 2	F_2S_2	(sulfur monofluoride) - 7
C_4H_8	(cis-2-butene) - 12	F_4OXe	(xenon oxyfluoride) - 7
C_4H_8O	(trans 2-3 epoxybutane) - 7	F_5I	(iodine pentafluoride) - 2
C_4H_8O	(tetrahydrofuran) - 2	F_5IO	(iodine oxide pentafluoride) - 25
$C_4H_{10}Br$	(t-butyl bromide) - 11	GeH_6Si	(silyl germane) - 7
C_5H_8	(cyclopentene) - 13	HBf_2	(difluoroborine) - 12

(continued FORMULA INDEX)

HNO_3 (nitric acid) - 7

HNSO (thionylimine) - 12

NO_2 (nitrogen dioxide) - 17

OS radical - 12

O_2S (sulfur dioxide) - 22, 10

H A R V A R D U N I V E R S I T Y

Department of Chemistry
12 Oxford Street
Cambridge 38, Massachusetts

June 16, 1964

Dear Contributor:

This is an addition to the microwave spectroscopy information letter:

THE UNIVERSITY OF BIRMINGHAM
Department of Chemistry

(John Sheridan)

CH_2FBr	Fluoro-bromomethane	P. Curnuck	Rotational and quadrupole assignment
$\text{C}_3\text{H}_3\text{F}$ (CH_2FCCH)	3-Fluoropropyne	B. E. Job	Carbon-13 species measured
$\text{C}_4\text{H}_5\text{D}$ ($\text{C}_2\text{H}_5\text{CCD}$)	Butyne-1-d	B. E. Job	Assigned
C_3IN	Iodo-cyanoacetylene	T. Bjorvatten	Constants in ground and excited states
C_3BrN	Bromo-cyanoacetylene	T. Bjorvatten	Constants in ground and excited states
$\text{C}_2\text{H}_4\text{N}_2$	Diazoethane	C. L. Dodson	Tentative assignment
C_2HF_3	Trifluoro-ethylene	O.L. Stiefvater	Assigned. Dipole moment. Tentative assignment of carbon 13 species.