

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

March 5, 1963

Dear Contributor:

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

1--ACADEMY OF SCIENCES OF THE USSR
P. N. Lebedev Physical Institute
(I. A. Mukhtarov)

$C_2H_3F_3$ (FH ₂ C-CHF ₂)	gauche 1-fluoro,2,2-difluoro ethane	manuscript prepared
$C_2D_3F_3$ (FD ₂ C-CDF ₂)	gauche 1-fluoro,1,1-di deutero,2,2-difluoro deutero ethane	manuscript prepared

2--UNIVERSITY OF BIRMINGHAM
Department of Chemistry
(John Sheridan)

CHDF.CN	fluoro-acetonitrile-d	B.E. Job	rotational constants assigned
CD ₂ F.CN	fluoro-acetonitrile-d ₂	B.E. Job	rotational constants assigned
CF ₂ H.CN	difluoro-acetonitrile	B.E. Job	rotational constants assigned
CH ₂ F.CCH	3-fluoro-propyne	B.E. Job	assignment of carbon-13 species in progress
CH ₃ .CH ₂ .CCH	butyne-1	B.E. Job	assigned, work on other species in progress
CD ₃ .Hg.Cl	methyl mercuric chloride-d ₃	P.Curnuck	assigned.

3--UNIVERSITY OF CALIFORNIA
Department of Chemistry
(W. D. Gwinn and R. J. Myers)

C_2H_5N	ethyleneimine	quadrupole and barrier paper in progress
C_3H_6S	trimethylene sulfide	assignment, including excited states
C_4H_6	cyclobutene	complete assignment
CF_3NO_2	trifluoronitromethane	paper in progress

(continued UNIVERSITY OF CALIFORNIA)

CH_3NO_2 (CH_3ONO)	methyl nitrite	work in progress
$\text{C}_4\text{H}_8\text{O}$	tetrahydrofuran	work in progress
$\text{C}_2\text{H}_6\text{O}$	dimethyl ether	accepted by J.C.P.
CH_3SF_5	methyl sulfurpentafluoride	paper in progress
IF_5	iodine pentafluoride	work in progress
BrF_5	bromine pentafluoride	work in progress
$\text{C}_4\text{H}_7\text{Cl}$	chlorocyclobutane	assigned
$\text{F}_3\text{CC:CCl}$	trifluoromethyl chloroacetylene	work in progress
$\text{C}_4\text{H}_6\text{O}$	dihydrofuran	assigned

4--COLUMBIA UNIVERSITY
Department of Chemistry
(B.P. Dailey)

$\text{C}_6\text{H}_5\text{Br}$	bromobenzene	Eli Rosenthal	manuscript being prepared
$\text{C}_6\text{H}_5\text{Cl}$	chlorobenzene	Eli Rosenthal	higher resolution measurements being made
$\text{C}_3\text{H}_5\text{Br}$	bromocyclopropane	M. K. Jam	spectrum partially analyzed

5--UNIVERSITY OF FREIBURG
Physikalisches Institut, Universität Freiburg i.Br.
(W. Maier)

$\text{C}_2\text{H}_6\text{OS}$ ($(\text{CH}_3)_2\text{SO}$)	dimethylsulfoxide	H. Dreizler u. G. Dendl	30 lines assigned, centrifugal distortion analy- sis underway
$\text{C}_3\text{H}_{12}\text{NB}$ ($(\text{CH}_3)_3\text{N}\rightarrow\text{BH}_3$)	trimethylamine- borane complex	H.-G. Schirde- wahn	several lines assigned
$\text{C}_3\text{D}_6\text{O}$ ($(\text{CD}_3)_2\text{CO}$)	acetone- d_6	F. Mönning	35 new lines assigned
CF_3NO	trifluoronitroso- methane	F. Mönning	dropped; no lines found

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

NO_2Cl	nitryl chloride(Stark effect)	D. Eagle	in manuscript
NOBr	nitrosyl bromide(Stark effect)	D. Eagle	in manuscript
SCl_2	thiophosgene	J. Murray	in progress

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

$\text{CH}_3\text{NO}(\text{CH}_2\text{NOH})$	formaldoxime	I. Levine	in press
$\text{C}_3\text{H}_7\text{S}(\text{CH}_3\text{CH}_2\text{CH}_2)$	propylene sulphide	S. Butcher	in press
$\text{C}_2\text{H}_4(\text{CH}_2\text{CO})$	ketone	A. Esbitt and P. Cox	in press
PH_2 (NSF)		W. Kirchhoff	manuscript ready
N_2F_2 cis		R. Kuczkowski	manuscript ready
HNSO		W. Kirchhoff	work completed
$\text{C}_3\text{H}_5\text{O}(\text{CH}_3\text{CH}_2\text{CHO})$	propionaldehyde	S. Butcher	work completed
$\text{C}_3\text{H}_3\text{F}(\text{CH}_2\text{FCH}:\text{CH}_2)$	3-fluoropropene	E. Hirota	work continuing in Tokyo
$\text{S}_2\text{F}_2(\text{SF}_2)$		R. Kuczkowski	assigned
$\text{C}_4\text{H}_8\text{O}(\text{CH}_3-\underset{\text{O}}{\text{CH}}-\text{CH}-\text{CH}_3)$	trans 2,3-epoxybutane	M. Emptage	work continuing
$\text{C}_2\text{H}_2\text{N}_2\text{C}(\text{CH}=\text{N}-\text{O}-\text{N}=\text{CH})$		E. Saegbarth	assigned

8--UNIVERSITY OF ILLINOIS
 Department of Chemistry
 (W.H. Flygare)

CD_3D	formaldehyde- D_2 (quadrupole)	experimental work completed
CH_3NCS	methyl isothiocyanate	} initial spectra taken. Start on the barrier calculations.
CH_3SCN	methyl thiocyanate	
Cl_2SiH_2	dichlorosilane	initial spectra taken
$\text{C}_2\text{H}_2\text{Cl}_2(\text{ClHC}:\text{CHCl})$	cis dichloroethylene	assignment on $\text{Cl}^{35,37}$ species. Other isotopic species are being searched for.
$\text{C}_2\text{H}_4\text{Cl}_2(\text{Cl}_2\text{HC}-\text{CH}_3)$	1,1-dichloroethane	two isotopic species assigned; barrier measurements being made.

Work has been suspended on C_5H_8 , methylene cyclobutane.

9--UNIVERSITY OF LOUVAIN
Institute for Nuclear and Molecular Physics
(M. de Hemptinne)

C_2H_5OH and C_2H_5OD	ethyl alcohol	J. Michielsens-Effinger	analysis in progress between 13. and 36kMc.
$CH_2 = CF_2$	vinylidène fluoride	J.C. Chauffoureaux	manuscript to appear in Bulletin de l'Académie Royale de Belgique
$S^{32}O_2^{18}$	sulfur dioxide	A. Defossez	work in progress between 13. and 30kMc.
$CHD=CHBr$ $CHD=CDBr$	bromures de vinyle	R. Windmolders	transitions 3-4 and 4-5 studied. Work on first excited level.
$S^{34}S^{16}O_2$ (excited states γ_2)	sulfur dioxide	R. Van Riet	will be published in "Annales de la Société Scientifique de Bruxelles"

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

$\underline{CH_2CH_2}CHCl$	cyclopropyl chloride	C-13, D, species nearly complete
$CH_3CHClCH_3$	2-chloropropane	nearly complete
$CH_3CHBrCH_3$	2-bromo-propane	Br-79, Br-81, C-13 species nearly complete
$\underline{OCH_2CH_2}OBH$	1,3,2-dioxaborodane	ground and first excited state species assigned.

11--NATIONAL BUREAU OF STANDARDS
Molecular Spectroscopy Section
(D. R. Lide)

$CH_3CH_2CH_2Cl$	<u>n</u> -propyl chloride	T. Sarachman	in press
$(CH_3)_3CCl$	<u>t</u> -butyl chloride	D. R. Lide	in press
$CH_2:CH C(CH_3):CH_2$	isoprene	D. R. Lide	spectrum assigned
ClO_3F	perchloryl fluoride	D. R. Lide	spectrum assigned
$HCOOH$	formic acid	T. Sarachman	almost complete
$CH_3CH:CHCH_3$	<u>cis</u> -2-butene	T. Sarachman	tentative assignment
CH_3CCSiH_3	methylsilylacetylene	D. R. Lide	spectrum assigned
AlF	aluminum monofluoride	D. R. Lide	in press
$LiCl$	lithium chloride	D. R. Lide	complete

12--NATIONAL RESEARCH COUNCIL
Division of Pure Physics
(C. C. Costain)

$\text{CH}_2:\text{CHCH}:\text{CHCN}$	1 cyano-1,3-butadiene	W.B. Dixon	1 conformation assigned
NH_2CN			
NHDCN	cyanamide	J. K. Tyler	several perturbed lines assigned, barrier calc.
ND_2CN			
CH_3OCl	methyl hypochlorite	S. S. Butcher	excited torsional states assigned.
$\text{C}_4\text{H}_8\text{S}$	tetrahydrothiophene	N. Posdeev	manuscript prepared

13--UNIVERSITY OF OKLAHOMA
Department of Physics
(Chun C. Lin)

CH_3SCN		Lin and Takahashi	Barrier height determined from doublets
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14--UNIVERSITY OF PADUA
Institute of Physical Chemistry
(Paolo G. Favero)

CHOF	formyl fluoride	A. Guarnieri	Zeeman effect: in press
NOCl	nitrosyl chloride	A.M. Mirri	millimeter wave spectrum. Centrifugal distortion analysis of a-type transitions: in press
			Search for b-type transitions in the 2 to 1 mm region
NOCl	nitrosyl chloride	P.G. Favero	nitrogen quadrupole coupling
CHCl_3	chloroform	A.M. Mirri	millimetre wave spectrum for centrifugal distortion analysis

15--QUEEN'S UNIVERSITY
Department of Physics
(David B. McLay)

CHFCl_2	dichlorofluoromethane		manuscript prepared
Impurity in CHFCl_2	not known		$J = 0 \rightarrow 1$ and Stark splitting measured

16--RICE UNIVERSITY
Department of Chemistry
(Robert F. Curl)

FNO	nitrosyl fluoride	centrifugal distortion work in progress
C ₂ H ₄ O ₂	acetic acid	isotopes prepared. Internal rotation reinvestigated. Work temporarily suspended
NO ₂	nitrogen dioxide	hyperfine parameters determined. manuscript in preparation

17--STANFORD UNIVERSITY
Department of Chemistry
(Victor W. Laurie)

C ₂ H ₇ N ((CH ₃) ₂ NH)	dimethylamine	J. Wollrab	manuscript in preparation
C ₂ H ₂ F ₂ (CH ₂ :CF ₂) (CHF:CHF)	vinylidene fluoride cis fluoroethylene	D. Pence	{manuscript in press, J. Chem. Phys.

18--UNIVERSITY OF STOCKHOLM
Institute of Physics
(H. Selén)

C ₆ H ₄ ClF	1-chloro-2-fluorobenzene	tentative assignments
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19--SWISS FEDERAL INSTITUTE OF TECHNOLOGY
Department of Physical Chemistry
(Hs. H. Günthard)

C ₂ H ₃ NO ₂ (CH ₂ :CHNO ₂)	nitro-ethylene	H.D. Hess	work in progress
C ₄ H ₆ O <u>CH₂-CH₂-CH₂-C=O</u>	cyclobutanone	A. Bauder	manuscript pre- pared for Helv. Phys. Acta

20--TECHNISCHE HOCHSCHULE KARLSRUHE
Institut für Physikalische Chemie
(Werner Zeil)

(CH ₃) ₃ SiCl	trimethylsilylchloride	H.K. Bodenseh	work in progress
CH ₃ COCCH	acetylacetylen	O. Stiefvater	work in progress

21--UNIVERSITY OF TOKYO
Department of Chemistry
(Yonezo Morino)

OCS carbonyl sulfide	}	C. Matsumura	spectra in the excited vibrational states assigned.	
OCS _e carbonyl selenide				
H ₂ CO formaldehyde	}	K. Takagi	spectra in the millimeter region, in manuscript, excited vibrational states.	
		T. Oka		
SO ₂ sulfur dioxide		Y. Kikuchi	spectra in the excited ν_1 and ν_2 states of S ³² O ¹⁶ ₂ , and ν_2 of S ³⁴ O ¹⁶ ₂ assigned, in manuscript.	
F ₂ CO carbonyl fluoride		S. Saito	spectra in the excited vibrational states assigned and analyzed.	
ClNO ₂ nitryl chloride	}	T. Oka	inertia defect, in press spectra in the excited vibrational states assigned.	
		T. Tanaka		
C ₆ H ₅ NO ₂ nitrobenzene		T. Oka	analysis in progress	
CHD=CH-CH ₂ F	}	3-fluoropropene	E. Hirota	spectra in the ground and torsional states of the cis and gauche forms assigned.
CH ₂ =CH-CHF				

22--Physical Laboratory, Utrecht, Holland
(H. A. Dijkerman)

C ₃ H ₄ O (HCCOCH ₃) methoxaethyn	spectrum found in region 17.5 - 39.5 KMc J = 1 → 2, J = 2 → 3 J = 3 → 4 assigned.
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23--West Virginia University
Department of Chemistry
(Jack D. Graybeal)

C ₂ H ₂ BrN(CH ₂ BrCN) bromoacetonitrile	R. Y. Lin	little additional progress since list of February, 1962.
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24--UNIVERSITY OF WISCONSIN
Department of Chemistry
(C. D. Cornwell)

CH ₃ F ₂ P (CH ₃ PF ₂) methyl difluorophosphine	E. A. Cohen	analysis in progress
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Sincerely,
C. Bright Wilson, Jr.
(pm)

FORMULA INDEX

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

AlF (aluminum monofluoride) - 11	C_2HD_2Br (vinyl bromide)-9
BrNO (nitrosyl bromide) - 6	$C_2D_3F_3$ (1-fluoro,1,1-di-deutero,2,2-difluoro deutero ethane) -1
CCl_2S (thiophosgene) - 6	$C_2H_3F_3$ (1 fluoro, 2,2-di-fluoro ethane) - 1
CF_2O (carbonyl fluoride) - 21	$C_2H_3NO_2$ (nitro-ethylene)-19
CF_3NO (trifluoronitrosomethane) - 5	C_2H_3NS (methyl thiocyanate)-8
CF_3NO_2 (trifluoronitromethane) - 3	C_2H_3NS (methyl isothiocyanate) -8,13
$CHCl_2F$ (dichlorofluoromethane) 15	$C_2H_4Cl_2$ (1,1-dichloroethane)-8
$CHCl_3$ (chloroform) - 14	$C_2H_4O_2$ (acetic acid) - 16
CHFO (formyl fluoride) - 14	$C_2H_5BO_2$ (1,3,2-dioxaborodane)-10
CH_2O (formaldehyde) - 21	C_2H_5N (ethyleneimine) - 3
CD_2O (formaldehyde - D_2) - 8	C_2H_6O (dimethyl ether) - 3
CH_2O_2 (formic acid) - 11	C_2H_6O (ethyl alcohol) - 9
CH_2N_2 (cyanamide) - 12	C_2H_6OS (dimethylsulfoxide) - 5
CD_3ClHg (Methyl mercuric chloride- d_3)-2	C_2H_7N (dimethylamine) - 17
CH_3ClO (methyl hypochlorite) - 12	C_3F_3Cl (trifluoromethyl chloroacetylene) -3
CH_3F_2P (methyl difluorophosphine)-24	C_3H_3F (3-fluoro-propyne) - 2
CH_3F_5S (methyl sulfurpentafluoride)-3	C_3H_4O (methoxaethyn) - 22
CH_3NO (formaldoxime) - 7	C_3H_4DF (3-fluoropropene) 21
CH_3NO_2 (methyl nitrite) - 3	C_3H_5Br (bromocyclopropane) - 4
COS (carbonyl sulfide) - 21	C_3H_5Cl (cyclopropyl chloride)-10
COSe (carbonyl selenide) - 21	C_3H_5F (3-fluoropropene) - 7
C_2HF_2N (difluoroacetonitrile) - 2	C_3D_6O (acetone- d_6) - 5
C_2H_2BrN (bromoacetonitrile) - 23	C_3H_6O (propionaldehyde) - 7
$C_2H_2Cl_2$ (cis dichloroethylene) - 8	C_3H_6S (propylene sulphide) - 7
C_2H_2DFN (fluoro-acetonitrile-d) - 2	C_3H_6S (trimethylene sulfide) -3
C_2D_2FN (fluoroacetonitrile- d_2) - 2	
$C_2H_2F_2$ (cis fluoroethylene) - 17	
$C_2H_2F_2$ (vinylidene fluoride) - 9,17	
$C_2H_2N_2O$ (<u>CH=N-O-N-CH</u>) - 7	
C_2H_2O (ketene) - 7	

C_3H_3Si (methylsilyl acetylene) - 11
 C_3H_7Br (2-bromo-propane) - 10
 C_3H_7Cl (2-chloropropane) - 10
 C_3H_7Cl (*n*-propyl chloride) - 11
 $C_3H_{12}NB$ (trimethylamine-borane complex) - 5
 C_4H_4O (acetylacetylene) - 20
 C_4H_6 (butyne - 1) - 2
 C_4H_6 (cyclobutene) - 3
 C_4H_6O (dihydrofuran) - 3
 C_4H_6O (cyclobutanone) - 19
 C_4H_7Cl (chlorocyclobutane) - 3
 C_4H_8 (cis-2-butene) - 11
 C_4H_8O (trans 2,3 epoxybutane)-7
 C_4H_8O (tetrahydrofuran) - 3
 C_4H_8S (tetrahydrothiophene) - 12
 C_4H_9Cl (*t*-butyl chloride) - 11
 C_5H_5N (1 cyano-1,3-butadiene) - 12
 C_5H_8 (isoprene) - 11
 C_6H_4ClF (1-chloro-2-fluoro-benzene)-18
 C_6H_5Br (bromobenzene) - 4
 C_6H_5Cl (chlorobenzene) - 4
 $C_6H_5NO_2$ (nitrobenzene) - 21
 $ClFO_3$ (perchloryl fluoride) - 11
 Cl_2H_2Si (dichlorosilane) - 8
 $ClLi$ (lithium chloride) - 11
 $ClNO$ (nitrosyl chloride) - 14
 $ClNO_2$ (nitryl chloride) - 6, 21
 FNO (nitrosyl fluoride) - 16
 FNS (NSF) - 7
 F_5Br (bromine pentafluoride) - 3
 F_5I (iodine pentafluoride) - 3

$HNOO$ - 7
 NO_2 (nitrogen dioxide) - 10
 N_2F_2 cis - 7
 O_2S (sulfur dioxide) - 21
 $O_2^{16}S^{34}$ (sulfur dioxide) - 9
 $O_2^{18}S^{32}$ (sulfur dioxide) - 9
 S_2F_2 (SSF_2) - 7
 $*C_3H_9ClSi$ (trimethylsilyl-chloride) - 20