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

October 19, 1961

Dear Contributor:

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

1-- AGRICULTURAL AND MECHANICAL COLLEGE OF TEXAS
Department of Chemistry
(Albert W. Jache)

SiF_3I	about finished
S_2Cl_2	14 lines measured

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

nitramide H_2NNO_2	(J.K. Tyler), (A-C) and asymmetry parameter assigned
cyanamide (NH_2CN)	(J.K. Tyler) Quadrupole coupling constants assigned from H_2NCH^{15} and $H_2N^{15}CN$
FCH_2CN	(B. Job) Assignment made of main species. Preliminary note sent for publication; other forms under investigation.
$FC^{13}N$ FCN^{15} $Cl^{35}CC^{13}H$ $Cl^{35}C^{13}CH$	(J.K. Tyler) B_o values determined. Paper in manuscript
HCCCCN, DCCCCN	(J.K. Tyler, A.P. Cox) D_J determined from mm-wave measurements
CH_3CF_3 CH_3SiF_3	(A.P. Cox) D_{JK}, D_J determined from mm-wave measurements
SiH_2DI SiH_2DBr^{79}, SiH_2DBr^{81} SiH_2DCl^{35}, SiH_2DCl^{37}	B_o, C_o evaluated (A.C. Turner)

(continued UNIVERSITY OF BIRMINGHAM)

$Si^{28}D_3I$	B_o, D_{JK} determined	(A.C. Turner)
$Si^{30}D_3I$	B_o determined	
SiH_3Cl^{35}	D_{JK}, D_J determined	
SiH_3CN	D_{JK} determined	
$SiH_3C^{13}N$	B_o determined	
SiD_3CN	B_o, D_{JK} determined	

3--UNIVERSITY OF CALIFORNIA
Department of Chemistry
(Rollie J. Myers, W. D. Gwinn, and J. A. Howe)

1,1-dichlorocyclopropane	preprints distributed
sulfur tetrafluoride	preprints distributed
formic acid (dipole moment)	revised note in progress
1,1-dichloroethane	assignment including quadrupole coupling
ethylenimine	quadrupole coupling measured (no inversion observed)
trimethylene sulfide	assignment including excited states
cyclobutene	Q-branch assignment
trifluoronitromethane	assignment confirmed-work in progress on barrier determination
methyl nitrite	assignment confirmed-work in progress
tetrahydrofuran	assignment confirmed-work in progress
IF_5	assignment-symmetric top
CH_3SF_5	assignment-symmetric top
cis-1,2-dichloroethylene	preprints to be distributed
1,1-dichloroethylene	strong field Stark effect
phosgene	strong field Stark effect
trans-1-chloro-2-fluoroethylene	work in progress

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

cyclobutylbromide	essentially complete
pyrimidine	partially complete
quadrupole coupling patterns in chlorobenzene	nearly finished

5--COLUMBIA RADIATION LABORATORY
(L. C. Krisher)

CH_3COI	in progress

6--UNIVERSITY OF COPENHAGEN
Chemical Laboratory
(Børge Bak)

benzonitrile	5 isotopic species prepared and analyzed. Three further species being prepared (^{13}C ring compounds).
furan	2-^{13}C and 3-^{13}C furans prepared. Not yet analyzed. Same for ^{18}O-furan
β-fluoronaphthalene	analyzed; being published
methyl ketene	The parent compound prepared, microwave analysis in good progress. So far, no isotopic work, but planned.

7--EMORY UNIVERSITY
Department of Chemistry
(J. H. Goldstein)

excited torsional states in acrolein	in progress
α-chloroacrylonitrile	in progress

8--UNIVERSITY OF FREIBURG
Institute for Physical Chemistry, Freiburg I.BR.
(W. Maier)

$(CH_3)_2S$	in progress, publication being prepared
$(CH_3)_2S_2$	in progress, assignment under way

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

$CHClF_2$	Rotational constants for $CHCl^{35}F_2$ and $CHCl^{37}F_2$ have been determined from low-J transitions. The spectrum of $CDClF_2$ will be studied in order to improve the structure determination. Dipole moment of $CHCl^{35}F_2$ has been measured by the Stark effect.
$CHFCl_2$ $SCCl_2$	Many lines have been detected. An attempt is being made to identify them.
NOBr	The Stark effect of the $1_1 \longrightarrow 2_0$ transition is being analyzed.

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

CH_2NOH	(I. Levine), in press
NSF_3	(W. Kirchhoff), in press
CH_3SnH_3	(P. Cahill and S. Butcher), in press
F_2O	(L. Pierce and R. Jackson) (See Notre Dame), in press
O_2F_2	(R. Jackson), in manuscript
CH_3CHCHF cis and trans	(R. Beaudet), in manuscript
$CH_3CH_2CH_2F$ trans and gauche	(I. Hirota), in manuscript
$CH_3CHCHCl$ trans	(R. Beaudet), work completed
CH_3OCl	(J. Rigden), analysis of several isotopes completed
CH_3CH_2CHO	(S. Butcher), analysis of several isotopes completed
GeH_3F	(J. Rigden), analysis of several isotopes completed
$CH_3CH_2CH_2CN$ trans and gauche	(I. Hirota), partially analyzed

(continued HARVARD UNIVERSITY)

GeH_3Br	(J. Rigden), partial analysis
$CF_3C_6H_5$	(T. Sarachman), partial analysis, no further work
cyclopentene	(G. Rathjens and A. Esbitt), new analysis completed
SNF	(W. Kirchhoff), early stages

11--UNIVERSITE LOUVAIN
Centre de Physique Nucleaire
(Robert Goedertier)

vinyl bromide	We have observed and attributed between 13.5 and 25.5 Gc the transition from J = 1 → 2 and J = 2 → 3 of 22 isotopic species (all the deuterated species, with carbon 12 and the two isotopes of bromine, and all the carbon 13 species with light hydrogen). The calculations for the determination of structure are presently in course.
sulphur dioxyde	(F. Greindl) The spectrum has been observed between 13 and 25.5 Gc at normal and dry ice temperature. The spectrum is attributed for the fundamental vibrational state with J up to 40 and some new lines for the $S^{34}O_2$. This work is carried out in view to investigate the first excited vibrational state.
ethyl alcohol	(J. Michielsen-Effinger) The spectra of C_2H_5OH and C_2H_5OD are observed in the 13 - 25.5 Gc range.
1.2 dibrom-ethylene	Earlier we tried to study this molecule, but no spectrum was observed.

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

ethylchloride, CH_3CH_2Cl	complete structure by the substitution method; work completed and manuscript submitted.

(continued MICHIGAN STATE UNIVERSITY)

chloromethylsilane, SiH_3CH_2Cl	complete structure by the substitution method, quadrupole coupling parameters, and barrier to internal rotation; work completed and manuscript submitted.
cyclopropyl chloride, CH_2CH_2CHCl	assignment made of C-type spectra of Cl-35 and Cl-37 species, work in progress on preparation of isotopic species.
isopropyl chloride, $(CH_3)_2CHCl$	work just getting underway.

13--NATIONAL BUREAU OF STANDARDS
(D. R. Lide, D. E. Mann, L. J. Nugent, T. N. Sarachman)

propylene(structure determination $(CH_3)_3CCCH$ and $(CH_3)_3CCN$ CH_3AsF_2	work completed, preprints already distributed.
$CHCl_3$(structure determination) $(CH_3)_3CCl$ " "	investigations substantially completed, but not yet written up.
$CH_2:CFCH:CH_2$(fluoroprene) $CH_2:C(CH_3)CH:CH_2$(isoprene) $CH_3CH_2CH_2Cl$ ClO_3F	problems now under active investigation on which significant progess has been made.
NF_2(spectrum not yet detected) CF_3NSF_2(tentative assignment)	other work in progress
CH_3CCl_3(isotopic species) C_3F_8(perfluoropropane) C_3F_6(perfluoropropylene) 1,3 butadiene(unsuccessful attempt made to detect spectrum of cis form)	problems investigated during last year but dropp because results were not promising.

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

acrolein, CH_2CHCHO	measurements completed on normal three C^{13} and O^{18} species Search for isomers not successful.
H-bonding, CF_3COOH-HCOOH and deuterated species	Note in press, J. Chem. Phys.
CF_3COOH-CH_3COOH	measurements of "symmetric-top" spectrum completed.

15--UNIVERSITY OF NOTRE DAME
Department of Chemistry
(Louis Pierce)

1,2,5 thiadiazole	(V. Dobyns), Common, d_2, ^{34}S, and ^{13}C species assigned. $^{2}H.F.S.$ partially resolved.
OF_2	(N. DiCianni, collaborating with R. Jackson of Harvard University), 17 ground state transitions assigned.
ethyl bromide	(C. Flanagan), Common species re-measured, isotopic species (^{13}C, ^{13}C, and 2 deuterated) prepared.
propyl silane	(J. Flood), Ground-state a-type and b-type transitions of trans species assigned.
ethyl methyl sulfide	(L. Pierce), Ground-state assigned (b-type) for both trans and gauche form.
ethyl methyl ether	(L. Pierce), Ground-state and several excited states assigned (b-type)for trans form.
dimethyl sulfide and dimethyl silane	(L. Pierce), Measurements on first-excited torsional state in progress.

16--UNIVERSITY OF PADUA
Institute of Physical Chemistry, Padua, Italy
(Paola G. Favero)

$FCl^{35}CO$	spectrum has been completed, paper to be submitted.

(continued UNIVERSITY OF PADUA)

$FCl^{37}CO$	almost complete and will shortly analyze the centrifugal distortion effect on relatively high J lines in the millimetre wave region.

17--RICE UNIVERSITY
Department of Chemistry
(R. F. Curl)

chlorine dioxide	manuscript submitted
formaldoxime	manuscript submitted

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

F_2CO	assignment made

19--Swiss Federal Institute of Technology
Zurich, Switzerland
(Hs. H. Gunthard)

cyclobutanone	spectra measured, partially analyzed
2-iodopropene	spectra measured, not analyzed
2-bromopropene	spectra measured, not analyzed
2-chloropropene	isotopes made
nitroethylene	spectra measured
azulene	spectra measured

20--TECHNISCHEN HOCHSCHULE KARLSRUHE, Germany
(Werner Zeil)

$(CH_3)_3CCl$	isotopes made and spectra measured
$(CH_3)_3CBr$	normal species partially analyzed
$(CH_3)_3SiCCH$ and $(CH_3)_3SiCCD$	compounds prepared
$(CH_3)_3CCCCl$	normal species investigated
$(CH_3)_3CCBr$ and $(CH_3)_3CCI$	prepared but no spectra yet
C_6H_5CCH	normal species investigated

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

CH_2CO	Papers for the molecules in the ground vibrational state have been published. Spectroscopy for the molecules in the vibrationally excited state is in progress. The spectra for the excited states of ν_3, ν_5, and ν_6 modes have been assigned.
SO_2	Spectral lines for the excited state of the ν_2 mode have been found. A number of lines of isotopic species have been assigned.
CD_3CN	Vibrationally excited lines were assigned. Anomaly of the ν_7 excited state was explained by the near degeneracy of ν_4 and ν_7.
trioxane $(CH_2O)_3$	Spectral lines of several vibrationally excited states have been found. C^{13} and O^{18} species were observed with the natural abundances and the structure of the ring has been determined.

I appreciate your cooperation and hope this list will prove useful.

Sincerely,

E Bright Wilson Jr

EBW:jm

E. Bright Wilson, Jr.

FORMULA INDEX

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

91

C_3H_4O (acrolein) - 7
C_3H_4O (CH_2CHCHO) - 14
C_3H_5Br (2-bromopropene) - 19
C_3H_5Cl ($CH_3CHCHCl$) - 10
C_3H_5Cl (CH_2CH_2CHCl) - 12
C_3H_5Cl (2-chloropropene) - 19
C_3H_5F (CH_3CHCHF) - 10
C_3H_5I (2-iodopropene) - 19
C_3H_6 (1,3-butadiene) - 13
C_3H_6 (propylene) - 13
C_3H_6O (CH_3CH_2CHO) - 10
C_3H_6O (trioxane $(CH_2O)_3$) - 21
C_3H_6S (trimethylene sulfide) - 3
C_3H_7Cl ($(CH_3)_2CHCl$) - 12
C_3H_7Cl ($CH_3CH_2CH_2Cl$) - 13
C_3H_7F ($CH_3CH_2CH_2F$) - 10
C_3H_8O (ethyl methyl ether) - 15
C_3H_8S (ethyl methyl sulfide) - 15
$C_3H_{10}Si$ (propyl silane) - 15
C_4HN (HCCCCN, DCCCCN) - 2
$C_4H_4N_2$ (pyrimidine) - 4
C_4H_4O (furan) - 6
C_4H_5F ($CH_2{:}CFCH{:}CH_2$) - 13
C_4H_6 (cyclobutene) - 3
C_4H_6O (cyclobutanone) - 19
C_4H_7Br (cyclobutylbromide) - 4
C_4H_7N ($CH_3CH_2CH_2CN$) - 10
C_4H_8O (tetrahydrofuran) - 3
C_4H_9Br ($(CH_3)_3CBr$) - 20
C_4H_9Cl ($(CH_3)_3CCl$) - 13
C_4H_9Cl ($(CH_3)_3CCl$) - 20
C_5H_8 (cyclopentene) - 10
C_5H_8 ($CH_2{:}C(CH_3)CH{:}CH_2$) - 13
C_5H_9Br ($(CH_3)_3CCBr$) - 20
C_5H_9I ($(CH_3)_3CCI$) - 20
C_5H_9N ($(CH_3)_3CCN$) - 13
$C_5H_{10}Si$ ($(CH_3)_3SiCCH$) and $(CH_3)_3SiCCD$) - 20
C_6H_5Cl (quadrupole coupling patterns in chlorobenzene)
C_6H_9Cl ($(CH_3)_3CCCCl$) - 20
C_6H_{10} ($(CH_3)_3CCCH$) - 13
$C_7H_5F_3$ ($CF_3C_6H_5$) - 10
C_7H_5N (benzonitrile) - 6
C_8H_6 (C_6H_5CCH) - 20
$C_{10}H_7F$ (β-fluoronaphthalene) - 6
$C_{10}H_8$ (azulene) - 19
$ClFO_3$ (ClO_3F) - 13
$Cl^{35}H_3Si$ (SiH_3Cl^{35}) - 2
$Cl^{35}DH_2Si$ (SiH_2DCl^{35}, SiH_2DCl^{37}) - 2
ClO_2 (chlorine dioxide) - 17
Cl_2S_2 (S_2Cl_2) - 1
DH_2ISi (SiH_2DI) - 2
D_3ISi^{28} ($Si^{28}D_3I$) - 2
D_3ISi^{30} ($Si^{30}D_3I$) - 2
FH_3Ge (GeH_3F) - 10
FNS (SNF) - 10
F_2N (NF_2) - 13
F_2O (F_2O) - 10
F_2O (F_2O) - 15
F_2O_2 (O_2F_2) - 10
F_3ISi (SiF_3I) - 1
F_3NS (NSF_3) - 10
F_4S (sulfur tetrafluoride) - 3
F_5I (IF_5) - 3
$H_2N_2O_2$ (nitramide H_2NNO_2) - 2
O_2S (SO_2) - 11
O_2S (SO_2) - 21