

Harvard University  
Department of Chemistry  
12 Oxford Street  
Cambridge, Massachusetts 02138  
U.S.A.  
Professor E. Bright Wilson

Michigan State University  
Department of Chemistry  
East Lansing, Michigan 48823  
U.S.A.

Professor Richard H. Schwendeman

May 16, 1974

Dear Contributor:

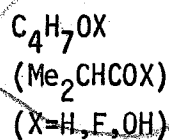
This is the seventeenth microwave spectroscopy information letter and is being sent to those who contributed. Apologies are due for the delay which arose from the use of surface mail in the invitational letters.

1. Institution: University College of North Wales, Bangor, Caerns., U.K.

Department: School of Physical and Molecular Sciences.

Name to whom queries should be addressed: John Sheridan

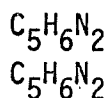
<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>INVESTIGATOR(s)</u>	<u>PRESENT STAGE</u>
CH <sub>3</sub> HgX (X=Cl, Br, I, CCH)	methyl mercury derivatives	C. Walls D.G. Lister	<sup>13</sup> C and D substitutions. r largely complete. Some α's.
C <sub>3</sub> H <sub>3</sub> NO	isoxazole	P. Nösberger O.L. Stiefvater	r <sub>s</sub> of ring. Continuing on D-substitution
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	imidazole	D. Christen	r <sub>s</sub> structure nearing completion. Refined coupling tensors.



isobutyric  
 aldehyde, acid,  
 acid fluoride

O.L. Stiefvater

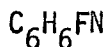
Study of rotational isomers  
 and structures continuing.



3-aminopyridine  
 4-aminopyridine

D. Christen  
 D.G. Lister  
 D. Norbury

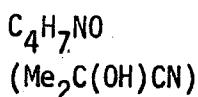
Amine deuterated species  
 assigned. MS prepared



o-fluoroaniline

D.G. Lister  
 D. Christen

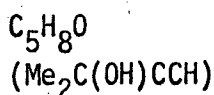
$O^+$  and  $O^-$  states of main  
 species assigned.



acetone  
 cyanohydrin

D.G. Lister

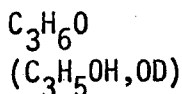
$\mu_a$  R-branch assignment of  
 normal species.



2-methyl-  
 3-butyne-2-ol

D.G. Lister

trial assignment



cyclopropanol

J.N. Macdonald  
 D. Norbury

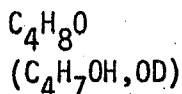
Work on gauche conformer  
 almost complete.



1-Me-cyclopropanol

C. Walls

trial assignment



cyclobutanol

J.N. Macdonald  
 D. Norbury

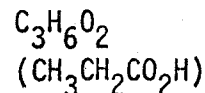
equatorial, OH/CH trans form  
 almost complete. Searching  
 for equatorial gauche.



cyclopent-3-ene-  
 1-ol

D.G. Lister  
 Miss S. Lowe

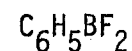
trial assignment



propionic  
 acid

O.L. Stiefvater

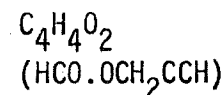
Study of gauche rotamer and  
 anomalies continuing.



phenyl boron  
 difluoride

D. Christen  
 D.G. Lister  
 D. Norbury

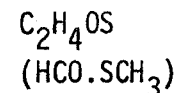
$^{10}B$  and  $^{11}B$  in ground and  
 torsional states assigned.  
 Barrier. MS prepared.



propargyl  
 formate

N.L. Owen  
 D.G. Lister

One rotamer assigned  
 (planar heavy atoms)



methyl  
 thioformate

N.L. Owen  
 D.G. Lister

assigned (in collaboration with  
 M.C.L. Gerry, U.B.C.)

2. Name of Institution Freie Universität Berlin  
 Name of Department or Institute Institut für Molekülphysik  
 Name to Whom Queries Should Be Addressed Prof. Dr. R. Honerjäger  
1000 Berlin 33  
Boltzmannstraße 20

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
BaO	Barium Oxide	J. Hoelt E. Tiemann T. Törring	to be published
OS <sub>2</sub> (S <sub>2</sub> O)	Disulfur Oxide		to be published in cooperation with NBS, Washington, D.C.
BrIn (InBr)	Indium Bromide		} hfs-structure assigned
BrRb (RbBr)	Rubidium Bromide		
BrCl	Bromine Chloride		
BrI (IBr)	Iodine Bromide		
BaS	Barium Sulfide	rotational spectrum assigned	
GeS	Germanium sulphide	} g <sub>J</sub> -factor and magnetic susceptibility anisotropy	
SnS	Tin sulphide		
PbS	Lead sulphide		
AlF	Aluminium monofluoride	} R.Honerjäger R.Tischer	Z.Naturforsch. 29a(1974)
FGa (GaF)	Gallium monofluoride		Manuscript in preparation
CuF	Copper monofluoride		
CsF	Cesium fluoride	} Ready for publication in Z.Naturforsch.	
ClCs (CsCl)	Cesium chloride		
BrCs (CsBr)	Cesium bromide		
CsI	Cesium iodide		

3. Name of Institution University of Bristol  
 Name of Department or Institute Department of Physical Chemistry, Bristol BS8 1TS  
 Name to Whom Queries Should be Addressed A. Peter Cox

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$\text{CH}_3\text{NO}$	nitrosomethane	P.H. Turner	Structure complete; centrifugal distortion in progress
$\text{CF}_3\text{NO}_2$	trifluoronitromethane	P.R.R. Langridge-Smith	Isotopic work in progress
$\text{C}_2\text{H}_6\text{F}_3\text{NSi}[\text{SiF}_3\text{N}(\text{CH}_3)_2]$	trifluorosilyl-dimethylamine	P.R.R. Langridge-Smith	Spectrum assigned
$\text{BF}_5\text{Si}[\text{SiF}_3\text{BF}_2]$	difluoro(trifluorosilyl) borane	T.Ogata	Barrier published
$\text{C}_7\text{H}_5\text{F}_3[\text{C}_6\text{H}_5\text{CF}_3]$	benzotrifluoride	T. Ogata	Spectrum assigned
$\text{BrF}_3\text{Si}[\text{SiF}_3\text{Br}]$	trifluorosilyl bromide	T.R. Gayton	Structure/ <u>dipole</u> /quadrupole coupling complete
$\text{C}_5\text{H}_5\text{NiNO}[\text{C}_5\text{H}_5\text{NiNO}]$	cyclopentadienyl nickel nitrosyl	I.C. Ewart	Excited states continuing
$\text{C}_5\text{H}_5\text{Tl}$	cyclopentadienyl thallium		
$\text{C}_8\text{H}_6$	phenyl acetylene	I.C. Ewart W.M. Stigliani	Structure/ <u>dipole</u> in manuscript

4. Name of Institution University of California, Santa Barbara, 93106  
 Name of Department Chemistry  
 Name to Whom Queries Should be Addressed David Harris (805)961-2534

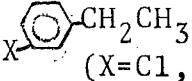
<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>INVESTIGATOR</u>	<u>STAGE</u>
CaF	Calcium Fluoride	Harris, Tanaka	Optical spectrum assigned; Microwave-Optical Double Resonance in progress.
$\text{NO}_2$	Nitrogen Dioxide	Tanaka	MODR-Manuscript in final stages


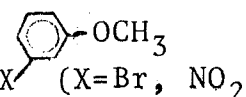
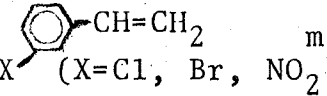
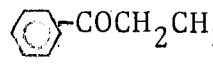
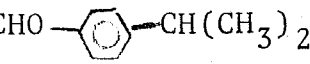
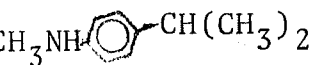
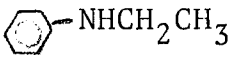
NaLi	Sodium Lithium	L. P. Gold	MODR begun
Oxaspiropentane		W. D. Slafer	5 isotopic species assigned

5. Name of Institution University of Chicago  
 Name of Department or Institute The James Franck Institute  
 Name to Whom Queries Should Be Addressed Donald H. Levy

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
NO <sub>2</sub>	Nitrogen Dioxide	Richard Solarz	Spectrum of <sup>2</sup> B <sub>2</sub> electronic state observed and partially assigned
OH	Hydroxyl radical	Antonie Churg	Analysis of v = 0 - 6 states almost complete
SeO	Selenium oxide	Shahla Butler	Magnetic resonance and microwave spectrum partly analyzed

6. Name of Institution: University of Connecticut, Storrs, Ct. 06268  
 Name of Department: Department of Chemistry  
 Name to Whom Queries Should Be Addressed: Robert K. Bohn

<u>Formula</u>	<u>Name of Compound</u>	<u>Name of Investigator</u>	<u>Present State of Progress</u>
 (X=Cl, Br, I)	m-Halo-Ethylbenzene	M. Farag	Low Resolution. Manuscript in Preparation

	p-Ethylbenzaldehyde	M. Farag	Low Resolution, Manuscript in Preparation
	m-X-anisole (X=Br, NO <sub>2</sub> )	M. Farag	Low Resolution Spectrum interpreted
	m-X-styrene (X=Cl, Br, NO <sub>2</sub> )	M. Farag	Low Resolution Spectrum interpreted
	Propiophenone	M. Farag	Low Resolution Spectrum interpreted
	p-i-Propylbenzaldehyde	M. Farag	Low Resolution Spectrum interpreted
	p-i-Propyl-N-methylaniline	M. Farag	Low Resolution Spectrum interpreted
	N-Ethylaniline	M. Farag	Low Resolution Spectrum interpreted
CF <sub>3</sub> COOR	Alkyl Trifluoro-methylacetate	N. True	Low Resolution
(R=CH <sub>3</sub> , CH <sub>2</sub> CH <sub>3</sub> , CH(CH <sub>3</sub> ) <sub>2</sub> , CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> )			
CHCl <sub>2</sub> CF <sub>2</sub> -O-CH <sub>3</sub>	2,2-Dichloro-1,1-difluoroethyl methyl ether	N. True	Low Resolution
CF <sub>3</sub> CH <sub>2</sub> -O-CH=CH <sub>2</sub>	2,2,2-Trifluoroethyl vinyl ether	N. True	Low Resolution

7. Institution: UNIVERSITY OF COPENHAGEN

Department: Chemical Laboratory V

Address: H. C. Ørsted Institutet  
DK-2100 Copenhagen

5, Universitetsparken  
DENMARK

FORMULA	COMPOUND	INVESTIGATOR	STATE OF PROGRESS
CH <sub>3</sub> NO (HCONH <sub>2</sub> )	formamide, -CD, -NHD, -ND <sub>2</sub> , - <sup>15</sup> N, - <sup>13</sup> C, - <sup>18</sup> O	Claus Nielsen Max Stubgaard +)G.O.Sørensen	Preliminary results (with E.Hirota), J.Mol.Spectrosc. 49(1974)251. Prep. of <sup>13</sup> C species in progress.

COS	$^{16}_O^{12}C^{32}_S$ $^{16}_O^{13}C^{32}_S$	+)N.W.Larsen	(with B.P.Winne- wisser, Kiel), vibr. satellites, mm-wave, in manu- script.
$C_2H_3N_3$	1,2,3-triazole 1-D species	+)G.O.Sørensen +)L.Nygaard M.Begtrup	In manuscript.
$C_3H_4N_2$	pyrazole	+)L.Nygaard et al.	J.Mol.Structure, in press.
$C_5H_5N$	pyridine	+)G.O.Sørensen et al.	J.Mol.Structure <u>20</u> (1974)119.
$C_5H_5NO$	pyridine N-oxide	Claus Nielsen Ole Snerling A.Tang-Pedersen +)G.O.Sørensen	Paper on ring-subst. species in progress. Prep. of D species in progress.
$C_5H_6$	1,2,4-pentatriene (vinylallene)	+)D.Christensen +)N.W.Larsen	a-type lines assigned.
$C_6H_5BrO$	4-Br-phenol	+)N.W.Larsen	In manuscript.
$C_6H_5ClO$	4-Cl-phenol	"	"
$C_6H_5FO$	4-F-phenol	"	"
$C_6H_5FS$	4-F-thiophenol-SD	+)N.W.Larsen +)T.Pedersen Leif Schulz	Barrier determined.
$C_6H_5NO_2$	nitrobenzene	Jens H. Høg +)G.O.Sørensen	Paper in progress.
$C_6H_6O$	phenol-OD	+)N.W.Larsen	(with Mathier et al.) J.Mol.Spectrosc. <u>47</u> (1973)183.
	phenol phenol-OD	"	Tors. and vibr. satellites, in manuscript.
	phenol- $^{13}C$	"	Complete $r_s$ structure, in manuscript.
$C_6H_6S$	thiophenol thiophenol-SD	+)N.W.Larsen +)T.Pedersen Leif Schulz	Barrier determined.

$C_6H_6Se$	selenophenol-SeD	+)N.W.Larsen Leif Schulz	a-type lines assigned.
$C_6H_7N$	aniline	Jens H. Høg +)N.W.Larsen	(with Lister et al.) J.Mol.Structure, in press.
$C_6H_7P$	phenylphosphine	+)N.W.Larsen T.Steinarrsson	a-type lines assigned.
$C_7H_5N$	phenylisocyanide	+)B.Bak et al.	J.Mol.Structure <u>18</u> (1973)429.
$C_8H_7Br$	Br-styrenes	+)L.Nygaard	Comment on broadband spectra, Acta Chem.Scand. <u>A28</u> (1974)118.

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+) Staff member.

8. Name of Institution Physikalisch-Chemisches Institut  
 Name of Department or Institute Justus Liebig-Universität Giessen, d-6300 Giessen  
 Name to Whom Queries Should Be Addressed Manfred Winnewisser

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$CHNO$ (HCNO, DCNO)	Fulminic Acid	M. Winnewisser and B.P. Winnewisser	Excited States manuscript in preparation
$C_3H_4O$ ( $CH_2CHCHO$ )	Acrolein	M. Winnewisser and G. Winnewisser	a-type and b-type MMW Spectrum analyse manuscript in preparation.
$C_2D_2O$ ( $D_2CCO$ )	dideteroketene	M. Winnewisser and L. Nemes	MMW Spectrum analysed




$C_2HDO$ ( $HDCO$ )	monodeuteroketene	" "	" manuscript in preparation.
$C_3H_3N$ ( $CH_2CHNC$ )	Vinylisocyanide	K. Yamada and M. Winnewisser	MMW spectrum assigned
$CHNO$ ( $HNCO$ )	Isocyanic acid all isotopic species	W.H. Hocking G. Winnewisser	Manuscript in preparation
$CH_3^{15}NO$ ( $CHO^{15}NH_2$ )	$^{15}N$ -Formamide	G. Winnewisser and W.H. Hocking	spectrum (MMW) assigned
$C_2H_3NO$ ( $CH_3CNO$ )	Methylfulmide	M. Winnewisser	MMW work will be started again.

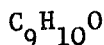
9. UNIVERSITY OF GLASGOW

DEPARTMENT OF CHEMISTRY

J. K. TYLER

$CN_2O$ ( $NO.CN$ )	Nitrosyl cyanide	R. Dickinson	$r_s$ structure complete. Dipole moment measured. NQHS and vib. state analyses in progress.
$C_8H_{10}S$ 	9-thia-bicyclo[3.3.1]-nona-2,6-diene	R. Dickinson	Main species assigned. Low lying vib. states being studied.
$C_6H_7N$ ( $C_6H_5NH_2$ )	aniline	J.K. Tyler (with J. Høg & N. Wessel-Larsen, U. of Copenhagen)	Paper in press. (J.Mol.Struct.)

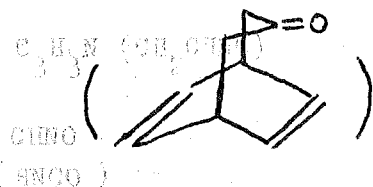
C<sub>9</sub>H<sub>10</sub>O (C<sub>9</sub>H<sub>10</sub>O)



Bicyclo[3.2.2]-nona-  
-6,8-diene-3-one

J.K. Tyler

Work in progress.



CH<sub>3</sub><sup>15</sup>NO (CH<sub>3</sub><sup>15</sup>NO)

10. Name of Institution University of Göteborg, Sweden

C<sub>2</sub>H<sub>5</sub>NO (C<sub>2</sub>H<sub>5</sub>NO)

Name of Department or Institute Department of Medical Physics

Name to Whom Queries Should Be Addressed Hasse Karlsson

<u>Formula</u>	<u>Name of Compound</u>	<u>Name of Investigator</u>	<u>Present Stage of Progress</u>
C <sub>2</sub> H <sub>5</sub> ClO	Chloromethyl-methyl ether	H.Karlsson	Manuscript submitted (with R.F.Curl and T. Ikeda, Rice Univ.)
C <sub>3</sub> H <sub>4</sub> F <sub>2</sub> O	1,3-Difluoroacetone	H.Karlsson	One rotamer assigned

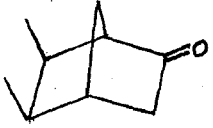
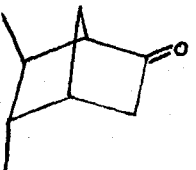
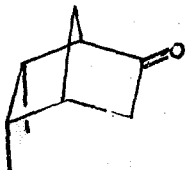
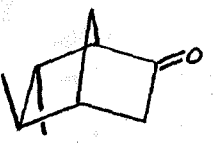
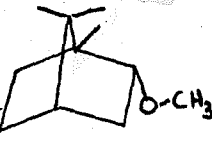
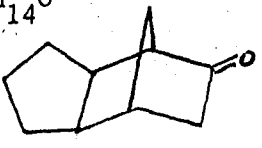
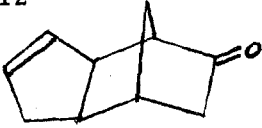
11. Name of Institution Harvard University

Name of Department or Institute Department of Chemistry

Name to Whom Queries Should Be Addressed E. Bright Wilson,

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>2</sub> H <sub>6</sub> S <sub>2</sub> (HSCH <sub>2</sub> -CH <sub>2</sub> SH)	1,2-Ethanedithiol	Steven Borchert	1 Gauche Conformer assigned.

$C_2H_2F_2O_3$ ( $F_2COOCH_2O$ ) 	1,1-difluoroethylene ozonide	Charles Gillies	Spectrum assigned.
$C_2H_2F_2O_3$ (HFCOOCHFO) 	cis- and trans- 1,2-difluoroethylene ozonide	Charles Gillies	Assignment in progress.
$C_4H_8O_3$ ( $CH_3CHOOCHCH_3O$ ) 	cis-2-butene ozonide	Charles Gillies	Assignment in progress.
$C_2H_5NO$ ( $CH_3CONH_2$ )	acetamide	Walter Rowe	A-torsional species assigned.
$C_3H_4O_2$ ( $O=CH-CH=CH-OH$ )	malondialdehyde	Walter Rowe	Assignment of isotopic species in progress.
$C_6H_8$	tricyclo(2.2.0.0 <sup>2,6</sup> )hexane	Richard Suenram	Normal species assigned & dipole moment determined. 3-deuterated species assigned & <sup>13</sup> C work in progress.
$C_3H_4F_2O$ ( $CH_2FCOCH_2F$ )	1,3-difluoroacetone	Richard Suenram David Finnigan Charles Gillies	cis-trans isomer assigned and dipole moment measured.
$C_{10}H_{17}Cl$	l-bornyl chloride	E. M. Bellott, Jr. Richard Suenram	Low resolution spectrum assigned.
$C_{12}H_{20}O_2$	l-bornylacetate	E. M. Bellott, Jr.	Conformational analysis in progress by low resolution microwave.
$C_{12}H_{18}O_2$	cis-2-acetoxypin-3-ene	E. M. Bellott, Jr.	Conformational analysis in progress by low resolution microwave.
$C_4H_7Cl$ ( $CH_2C(CH_3)CH_2Cl$ )	isobutenyl chloride	D. Finnigan	Completed.
$C_3H_4ClN$ ( $ClCH_2CH_2CN$ )	3 chloropropionitrile	I. Warren	Completed.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_9H_{14}O$ 	exo,exo-5,6-dimethyl-norcamphor	E. M. Bellott, Jr.	Low resolution spectra observed. These four isomeric compounds have been distinguished by low resolution spectroscopy.
$C_9H_{14}O$ 	endo-exo		
$C_9H_{14}O$ 	endo-endo		
$C_9H_{14}O$ 	exo-endo		
$C_{11}H_{20}O$ 	l-bornyl-methyl ether	E. M. Bellott, Jr.	Low resolution spectrum attempted, not observed.
$C_{10}H_{14}O$ 	8-ketotricyclo[5.2.1.0 <sup>2,6</sup> ]decane	E. M. Bellott, Jr.	Low resolution microwave spectrum observed.
$C_{10}H_{12}O$ 	8-ketotricyclo[5.2.1.0 <sup>2,6</sup> ]-4-decene	E. M. Bellott, Jr.	Low resolution microwave spectrum observed.
$C_4H_7N$ ( $CH_3CH_2CH_2NC$ )	n-propyl isocyanide	M. Fuller	2 forms assigned.
$C_3H_6O$ ( $CH_3CH_2CHO$ )	propanal	D. Scroggin H. Pickett	Being submitted.
$C_3H_7ClO$ ( $C\&CH_2CH_2CH_2OH$ )	chloropropanol	M. Fuller	2 forms assigned.

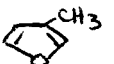

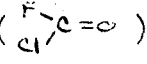
12. Name of Institution University of Kansas  
 Name of Department or Institute Department of Chemistry  
 Name to Whom Queries Should Be Addressed Marlin D. Harmony

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$\text{CH}_4\text{NO}(\text{CH}_3\text{ONH}_2)$	Methoxyamine	Fong	Manuscript submitted
$\text{C}_6\text{H}_7\text{N}(\text{NC}-\text{C}_4\text{H}_6-\text{CH}_2)$	Methylene cyclobutyl cyanide	Fong with Durig	In press
$\text{N}_2\text{D}_4$	Hydrazine	Baron	Spectral and theoretical work
$\text{C}_6\text{H}_{10}(\text{CH}_3-\text{C}_{10}\text{H}_{16})$	2-methyl bicyclo[2.1.0]pentane	Harmony	Endo and exo-isomers
$\text{C}_3\text{H}_7\text{N}(\text{C}_3\text{H}_5\text{NH}_2)$	Cyclopropylamine	Bostrom	$\text{C}^{13}$ species
$\text{C}_7\text{H}_{10}\text{O}(\text{C}_{10}\text{H}_{16}\text{O})$	Norbornanone	Yu	Studied as tool for photochemical studies.
$\text{C}_6\text{H}_8(\text{C}_{10}\text{H}_{16})$	Bicyclo[2.1.1]hex-2-ene	Harmony	In progress

13. Name of Institution: Universität Kiel, 23 Kiel, W. Germany

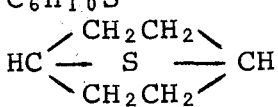
Name of Department or Institute: Abt. Chemische Physik, Institut f. Physikalische Chemie

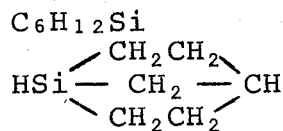
Name to whom queries should be addressed: Helmut Dreizler

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
$C_3H_5N$ ( $CH_3CH_2CN$ )	propionitrile	H. Heise, H. Lutz, H. Dreizler	$r_s$ -Structure; torsion-vibration- rotation-interaction
$C_2D_3H_3S_2$ ( $(^2CD_3SSCH_3)$ )	trideuteromethyl- methyl disulfide	M. Kuhler	Torsion-vibration- rotation-interaction (manuscript prepared)
$C_2H_3SN$ ( $CH_3SCN$ )	methyl thiocyanate	U. Andresen	Torsion-vibration- rotation-interaction (manuscript prepared)
$C_3H_5FO$ ( $CH_2FCCH_3$ )	Fluoroacetone	U. Andresen	Torsion-vibration- rotation-interaction
$C_5H_6O$ (  )	3-methylfuran	W. Czieslik	Zeeman studies
$C_6H_4F_2$ (  )	1,3-difluorobenzene	J. Wiese	Zeeman studies
$CH_3BF_2$	methyl boron difluoride	L. Engelbrecht	Zeeman studies
$CH_3NO_2$	nitromethane	L. Engelbrecht	Zeeman studies
$C_2H_6N_2O$ ( $(^2(CH_3)_2NNO)$ )	dimethylnitrosamine	F. Rohwer, A. Guarnieri	$r_s$ -Structure
$C_2H_6N_2O_2$ ( $(^2(CH_3)_2NNO_2)$ )	dimethylnitramine	A. Guarnieri, F. Scappini	Measurement in progress
$CH_3SCl$	methane sulfenyl chloride	A. Guarnieri	Torsion-vibration- rotation-interaction
$COFCl$ (  )	carbonylfluoro chloride	A. Guarnieri, F. Scappini, E. Hamer	Zeeman studies

D <sub>2</sub> CCO	dideuteroketene	K.V.L.N. Sastry, A. Guarnieri	Zeeman effect, sign of dipole moment
HOCl	hypochloric acid	A. Guarnieri, F. Scappini	Zeeman studies
NOF	nitrosyl fluoride	A. Guarnieri, H. Dreizler	Zeeman studies

14 Name of Institution Kyushu University, JAPAN  
Name of Department Department of Chemistry, Faculty of Science  
Name to Whom Queries Should Be Addressed Eizi Hirota

Formula	Name of Compound	Name of Investigator	Present Stage of Progress
C <sub>5</sub> H <sub>8</sub> [CH <sub>2</sub> =CHCH <sub>2</sub> CH=CH <sub>2</sub> ]	1,4-Pentadiene	T. Shigemune E. Hirota	One rotamer assigned.
O <sub>2</sub>	Oxygen	T. Amano	Manuscript submitted.
CH <sub>3</sub> F, CD <sub>3</sub> F	Methyl fluoride	T. Tanaka	Manuscript in preparation.
C <sub>6</sub> H <sub>10</sub> S 	7-Thiabicyclo [2.2.1]heptane	K. Irie E. Hirota	Work in progress.
CH <sub>3</sub> Cl, CD <sub>3</sub> Cl	Methyl chloride	M. Hirashita	Manuscript in preparation.
ClHO <sub>4</sub> (HOClO <sub>3</sub> )	Perchloric acid	K. Fujimoto	Assigned.
CH <sub>2</sub> F <sub>2</sub> , CD <sub>2</sub> F <sub>2</sub>	Methylene fluoride	E. Hirota M. Sahara	Work completed.
ClO	Chlorine monoxide	T. Amano	Manuscript in preparation.
C <sub>3</sub> H <sub>8</sub> O, C <sub>3</sub> H <sub>7</sub> OD [(CH <sub>3</sub> ) <sub>2</sub> CHOH, (CH <sub>3</sub> ) <sub>2</sub> CHOD]	Isopropanol	E. Hirota	Work in progress.



1-Silabicyclo  
[2.2.1]heptane

K. Tanaka  
T. Ikeura

Assigned.

$\text{F}_2\text{S}(\text{SF}_2)$

Sulfur difluoride

T. Chikaraishi

Work completed.

$\text{F}_4\text{S}(\text{SF}_4)$

Sulfur tetrafluoride

H. Inoue

Excited vibrational states; Assigned.

$\text{C}_3\text{H}_4\text{O}$

Acrolein

T. Honda

Centrifugal distortion; Work completed.

$\text{C}_3\text{H}_4\text{F}_2$

3,3-Difluoropropene

I. Botskor

Two rotamers assigned.

$\text{CH}_4(\text{CH}_2\text{D}_2)$

Methane

E. Hirota  
M. Hirashita

Assigned.

15. Name of Institution University of Manchester

Name of Department or Institute Schuster Laboratory

Name to Whom Queries Should Be Addressed Dr. J. G. Baker

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
Example: $\text{CH}_4\text{O}(\text{CH}_3\text{OH})$	Methyl alcohol	John Doe	Spectrum assigned
$\text{Br F}_5$	Bromine pentafluoride	S. R. Jones	Paper on excited states in preparation
$\text{IF}_5$	Iodine pentafluoride	S. R. Jones	Excited states in progress
$\text{PO Cl}_3$	Phosphorus trichloride	G. C. Georghiou	Quadrupole analysis



16. Name of Institution University of Maryland

Name of Department or Institute Institute for Molecular Physics

Name to Whom Queries Should Be Addressed Lawrence C. Krisher

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$\text{CH}_5\text{GeF}(\text{CH}_2\text{FGeH}_3)$	Fluoromethyl-germane	L. C. Krisher W. A. Watson	Manuscript submitted.
$\text{CF}_3\text{GeH}_3$	Trifluoromethyl-germane	L. C. Krisher W. A. Watson	In progress.

17. Name of Institution Massachusetts Institute of Technology

Name of Department or Institute Department of Chemistry

Name to Whom Queries Should Be Addressed Professor S. G. Kukolich

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$\text{BrCH}_3(\text{CH}_3\text{Br})$	Methyl Bromide	J. Williams	Some High Resolution Spectrum Obtained
$\text{CH}_4\text{O}(\text{CH}_3\text{OH})$	Methyl Alcohol	K. Casleton	Maser spectra of K=2+3 transitions and Zeeman work

COS (OCS)	Carbonyl Sulphide	P. Foreman, K.R. Chien	Relaxation cross-sections obtained
FNO	Nitrosyl Fluoride	S.G. Kukolich	Maser spectra obtained

18. Name of Institution Memphis State University

Name of Department or Institute Chemistry Department

Name to Whom Queries Should Be Addressed Robert G. Ford

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>6</sub> O	3-butyn-1-ol	L. Szalanski	hydrogen bonded form assigned
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	3-cyanopyridine	R. Ford	spectrum assigned
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	4-cyanopyridine	R. Ford	spectrum assigned
C <sub>2</sub> H <sub>2</sub> ClFO	fluoroacetyl chloride	L. Szalanski	Manuscript in preparation
C <sub>2</sub> H <sub>3</sub> ClO	chloroacetaldehyde	R. Ford	two rotamers assigned
C <sub>5</sub> H <sub>8</sub>	1,2-pentadiene	R. Ford	two rotamers assigned

19. Name of Institution: Michigan State University

Name of Department or Institute: Department of Chemistry

Name to Whom Queries should be Addressed: Richard H. Schwendeman

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STATE OF PROGRESS
$C_3H_4O_2$ ( $CH_2OCHCHO$ )	Glycidaldehyde	P. Manor R. Assink	Manuscript in preparation
$C_4H_8O$ ( $CH_3CH_2CH_2CHO$ )	n-Butyraldehyde	P. Lee	Two rotamers Manuscript in preparation
$CH_3F_2P$ ( $CH_3PF_2$ )	Methyldifluorophosphine	E. Coddling R. Creswell	In press
$CH_6BF_2P$ ( $CH_3PF_2BH_3$ )	Methyldifluorophosphine-BH <sub>3</sub>	R. Creswell R. Elzaro	Normal and BD <sub>3</sub> species assigned
$C_3H_7NO$ ( $HCON(CH_3)_2$ )	Dimethylformamide	S. Brown A. Brittain R. Elzaro	Parent, d <sub>7</sub> , and CD <sub>3</sub> (cis and trans) species assigned
$C_2H_5NO$ ( $HCONHCH_3$ )	N-methylformamide	R. Creswell R. Elzaro	Species with CH <sub>3</sub> cis to O assigned
$C_2H_4O$ ( $CH_2CH_2O$ )	Ethylene oxide	R. Creswell	<sup>17</sup> O quadrupole Manuscript in preparation

20. Name of Institution The University of Michigan

Name of Department or Institute Department of Chemistry

Name to Whom Queries Should Be Addressed Dr. Robert L. Kuczkowski

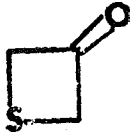

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_5H_5As$	arsabenzene	R. Lattimer	Manuscript in prep


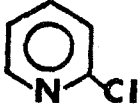




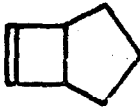
$C_2H_3FO_3$ (FH $\overline{COOCH_2O}$ )	1-Fluoroethylene ozonide	R. Lattimer	Assigned
HNSOF <sub>2</sub> (HN = S(O)F <sub>2</sub> )	imidosulfuryl fluoride	P. Cassoux	Assigned
(CH <sub>3</sub> ) <sub>3</sub> NBH <sub>3</sub>	trimethylamine borane	P. Cassoux	<sup>15</sup> N species
C <sub>5</sub> H <sub>4</sub>	1,4 pentadiyne	R. Lattimer	2 isotopes assigned
C <sub>2</sub> H <sub>4</sub> O <sub>3</sub> (H <sub>2</sub> $\overline{COOCH_2O}$ )	Ethylene ozonide	R. Kuczkowski	Further studies on deuterated species
N <sub>2</sub> O <sub>3</sub>	Dinitrogen Trioxide	R. Kuczkowski	Vib. Sat. No progress since last newsletter

21. Name of Institution Mississippi State University

Name of Department or Institute Department of Physics

Name to whom Queries should be Addressed R. L. Cook or T. B. Malloy, Jr. or G. E. Jones

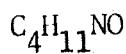
<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>3</sub> H <sub>2</sub> N <sub>2</sub> CH <sub>2</sub> (CN) <sub>2</sub>	methylene cyanide (malononitrile)	Centrifugal distortion analysis complete for J up to 62.
C <sub>3</sub> H <sub>4</sub> OS	 thietanone-3	Spectrum assigned in ground state and 10 excited states of ring-puckering mode, potential function determined. MS in prep.
C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	 2,3-dihydro-p-dioxin (1,4-dioxene)	In Press, J. Chem. Phys.

$C_4H_8OS$		1,4-thioxane	Spectrum assigned, Stark effect measurements completed, analysis near complete, MS in progress
$C_5H_4ClN$		2-chloropyridine	In Press, J. Mol. Spectrosc.
$C_5H_8O$		3,6-dihydro-2H-pyran	In Press, J. Chem. Phys.
$C_5H_8O$		3-oxabicyclo(3.1.0.)hexane	In Press, J. Mol. Spectrosc.
$C_6H_8$		1,2-dimethylenecyclobutane	Spectrum assigned in ground state and 4 excited states, Stark effect measurements completed.
$C_6H_{10}$		bicyclo(3.1.0.)hexane	In Press, J. Amer. Chem. Soc.
$C_7H_{10}$		$\Delta$ bicyclo(3.2.0.)heptene	Spectrum assigned, Stark effect measurements completed, analysis in progress.

22. Name of Institution The University of Missouri-St. Louis  
 Name of Department or Institute Chemistry Department  
 Name to Whom Queries Should Be Addressed Robert E. Penn

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_9NO$	2-methylaminoethanol	Buxton	Two hydrogen bonded rotamers assigned rel. energy determined

*Handwritten notes:*  
 $CH_3$   $H$   $OH$   
 $CH_2$



2-dimethylaminoethanol Birkenmeier

Hydrogen bonded rotamer assigned




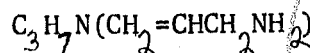
cyclopropyl cyanide Penn

Structural work begun at the Univ. of Texas at Austin with James E. Boggs - nearly completed.

MONASH UNIVERSITY, AUSTRALIA.....See # 54.

23. Name of Institution University of Nancy  
 Name of Department or Institute Laboratoire de Chimie Theorique, Case Officielle n° 140  
 Name to Whom Queries Should Be Addressed G. Roussy; J. Barriol

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_4H_5NS(CH_2=CHCH_2NCS)$	Allylisothio-cyanate	A. Bouchy	Work in progress
$C_7H_5NO(C_6H_5NCO)$	Phenyliso-cyanate	A. Bouchy	Excited Vibrational states assigned
$C_7H_5NS(C_6H_5NCS)$	Phenylisothio-cyanate	A. Bouchy	Spectrum assigned
$C_7H_8$ 	Toluene	J. J. Masini	$^{13}C$ species, analytical uses
$C_6H_5Cl$	Chlorobenzene	F. Michel H. Nery	$r_s$ structure nearly completed; Excited vibrational states assignment; Multiple substitutions



Allylamine

G. Roussy  
in collaboration  
with Freiburg

Search for a third  
rotamer with D.R.

24 Name of Institution National Bureau of Standards  
Name of Department or Institute Molecular Spectroscopy Section  
Name to Whom Queries Should Be Addressed Donald R. Johnson

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
AB	Diatomic Molecules	Lovas, Tiemann*	Tabulation of Microwave Data
COS	Carbonyl sulfide	Maki	Vibrational excited states for <sup>34</sup> S isotope
C <sub>2</sub> H <sub>5</sub> N(CH <sub>3</sub> CH=NH)	<u>trans</u> -C-Methyl Methyleneimine	Johnson, Lovas Clark	Spectrum Observed and partially assigned
C <sub>2</sub> H <sub>5</sub> N(CH <sub>3</sub> CH=NH)	<u>cis</u> -C-Methyl Methyleneimine	Clark, Johnson Lovas	Spectrum assigned, further measurements in progress
C <sub>2</sub> H <sub>5</sub> N(CH <sub>2</sub> =CHNH <sub>2</sub> )	Vinylamine	Lovas, Clark Tiemann*	Hyperfine structure, dipole moment, partial structure. Manuscript in preparation
OS (SO)	Sulfur Monoxide	Tiemann*	J. Mol. Spectrosc. J. Phys. Chem. Ref. Data
OS <sub>2</sub> (S <sub>2</sub> O)	Disulfur Monoxide	Tiemann*, Hoefft Lovas, Johnson	Structure and centrifugal distortion. Submitted to J. Chem. Phys.
O <sub>2</sub> S <sub>2</sub> (OSSO)	SO-Dimer	Lovas, Tiemann* Johnson	Structure, centrifugal distortion, dipole moment. Submitted to J. Chem. Phys.

\* On sabbatical from the Free University, Berlin, 1973.

25. Name of Institution University of New Brunswick  
Name of Department or Institute Physics and Chemistry  
Name to Whom Queries Should Be Addressed K.V.L.N. Sastry (PHYSICS)

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_6O_2$ ( $\overbrace{CH_2-O-CH-CH_2OH}$ )	Glycidol	W.V.F. Brooks and K.V.L.N. Sastry	-OH and -OD spectra assigned

26. Name of Institution University of New Orleans  
Name of Department or Institute Department of Physics - New Orleans, LA 70122  
Name to Whom Queries Should Be Addressed E. L. Beeson

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_6H_2F_4$	1-2-3-4 Tetrafluorobenzene	S.N. Mathur	Ground state assigned



27. Name of Institution: University of Newcastle upon Tyne, U.K.

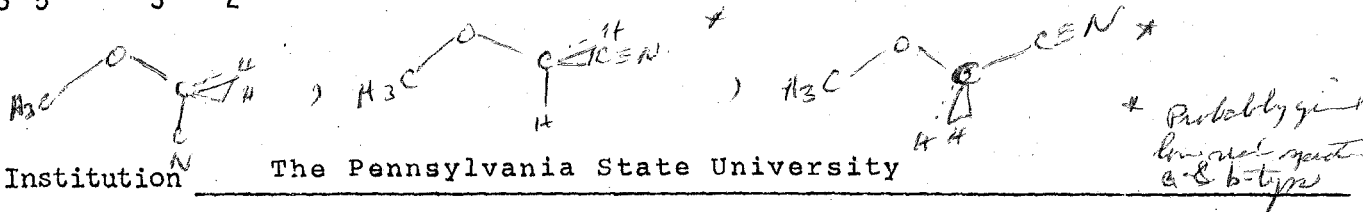
Name of Department: Physical Chemistry Department

Name to Whom Queries should be addressed: Professor D.H. Whiffen

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
COBr <sub>2</sub>	Carbonyl bromide	I. Thompson	Centrifugal Distortion Analysis
CSCl <sub>2</sub>	Thiocarbonyl chloride	D.F. Rimmer	Manuscript in Preparation
CSBr <sub>2</sub>	Thiocarbonyl bromide	I. Thompson	Temporarily abandoned
ClNO	Nitrosyl chloride	J.H. Carpenter	Excited Vibrational States
FNO	Nitrosyl fluoride	D.F. Rimmer	Excited Vibrational States
F <sub>3</sub> PO	Phosphoryl fluoride	J.G. Smith	Assignment of degenerate vibrational states in progress

28. Name of Institution University of Oslo  
 Name of Department or Institute Department of Chemistry  
 Name to Whom Queries Should Be Addressed K.-M. Marstokk/ H. Møllendal

<u>FORMULA</u>	<u>Name of COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_2H_2O_3(CHOCO_2H)$	Glyoxylic acid	J.Christiansen	5 isotopic species assigned
$C_2H_6O_2(CH_2OHCH_2OH)$	Ethylene glycol	H.Møllendal	In press
$C_2H_4FNO(CH_2FCONH_2)$	2-Fluoroacetamide	H.Møllendal	In press
$C_5H_5NO$	Pyrrole-2-carbox-aldehyde	H.Møllendal	In press
$C_3H_5NO(CH_3OCH_2CN)$	Methoxyacetonitrile	K.Solgaard	Abandoned



29. Name of Institution The Pennsylvania State University  
 Name of Department or Institute Chemistry Department  
 Name to Whom Queries Should Be Addressed Prof. L. Peter Gold

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$CH_5As(CH_3AsH_2)$	methyl arsine		paper in preparation
$C_2H_7As((CH_3)_2AsH)$	dimethylarsine		paper in preparation
$LiNa$	sodium lithium		preliminary experiments begun at U. Cal. Santa Barbara on microwave-optical double resonance

30. Name of Institution Princeton University  
Name of Department or Institute Department of Chemistry  
Name to Whom Queries Should Be Addressed Victor W. Laurie

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_4F_2$	1,1-difluorocyclopropane	A. Peretta	Manuscript in preparation
$C_4H_5N$	cyclopropylcyanide	R. Pearson	Manuscript in preparation
$C_5H_4N_2$	1,1-dicyanocyclopropane	R. Pearson and A. Choplin	Assigned
$C_3H_4$	cyclopropene	W. Stigliani	Two $^{13}C$ species assigned, centrifugal distortion analysis carried out
$C_3H_2F_4$	tetrafluorocyclopropane	W. Stigliani	Two isotopic species assigned
$C_2H_7N$	ethylamine	Y. S. Li	Manuscript in preparation

31 Name of Institution Queen's University at Kingston, Ontario, Canada  
Name of Department or Institute Department of Physics  
Name to Whom Queries Should Be Addressed Dr. D.B. McLay

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
OH, OD	Hydroxyl radical	Jaime Bigu and D.B. McLay	Stark-modulated epr spectrum at 13.65 GHz measured and analyzed

32. Name of Institution Queen's University, Kingston, Ontario, Canada

Name of Department or Institute Chemistry

Name to Whom Queries Should Be Addressed R. Kewley

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_5H_{11}NO$	N-methyl morpholine	S.C. Dass	In press
$C_5H_8O$	1-methoxybutadiene	S.C. Dass	Initial assignment
$C_6H_{12}O$	Oxepane	S.C. Dass	Complex spectrum observed
$C_6H_{13}N$	N-methyl piperidine	S.C. Dass	work suspended
$C_5H_{11}N$	Piperidine (axial NH)	R.S. Lowe	Centrifugal distortion
$C_4H_8O_2$	1,3-dioxane	R.S. Lowe	fits for high J Q-branches
$C_5H_{10}O$	Tetrahydropyran	R.S. Lowe	J Q-branches
$C_3H_5NO$	Methoxyacetonitrile	R. Kewley	In press
$C_5H_{10}N_2$	Tert-butyl cyanamide	R. Kewley	Assignment in progress

33. Name of Institution: University of Reading, Berkshire, England

Name of Department or Institute: Department of Chemistry

Name to Whom Queries Should be Addressed: Ian M Mills

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$CH_3I$	Methyl Iodide	P D Mallinson	Manuscript in preparation.
	$CH_2DI$		
$C_3H_6O$	Oxetane- $\alpha$ $_2$	P D Mallinson A G Robiette	Manuscript submitted

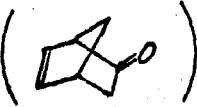
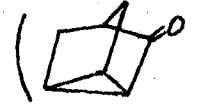



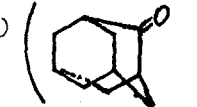
CH <sub>3</sub> Cl	Methyl Chloride CHD <sub>2</sub> <sup>35</sup> Cl CHD <sub>2</sub> <sup>37</sup> Cl	P D Mallinson	Most of spectrum assigned, rotational constants determined.
C <sub>2</sub> H <sub>3</sub> N (CH <sub>3</sub> CN)	Methyl Cyanide CHD <sub>2</sub> CN	P D Mallinson	Many ground state lines assigned. Assignment of excited vibrational states in progress.
CH <sub>3</sub> NO <sub>2</sub>	Nitromethane	P D Mallinson J A Duckett	Many ground state lines assigned. Rotational constants, barrier and distortion constants determined. Excited vibrational states.
C <sub>5</sub> H <sub>10</sub> O	3,3-Dimethyl Oxetane	J A Duckett	Assignment in progress. Excited vibrational states.

34. Name of Institution Rice University  
 Name of Department or Institute Chemistry Department  
 Name to Whom Queries Should Be Addressed R. F. Curl

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH <sub>6</sub> OSi	Silyl Methyl Ether	C. D. LeCroix	Manuscript Submitted
C <sub>2</sub> ClH <sub>5</sub> O	Chloromethyl Methyl Ether	T. Ikeda	Manuscript Submitted
C <sub>3</sub> FH <sub>3</sub> O	Acryloyl Fluoride	R. S. Williams	Measurements on <u>cis-trans</u> energy difference
C <sub>3</sub> H <sub>9</sub> NO	3-Amino Propanol	M. Norris	Normal, 3 D species assigned. Dipole Measured

$C_4H_6O$	Butadiene Monoxide	T. Ikeda, K. V. L. N. Sastry	Manuscript in Preparation
$HNO_2$	Nitrous Acid	R. Varma	Measurements on <u>cis-trans</u> energy difference

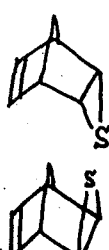
35. Name of Institution San Diego State University, San Diego, California 92115  
 Name of Department Chemistry  
 Name to Whom Queries Should Be Addressed Dewitt Coffey, Jr.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>PRESENT STAGE OF PROGRESS</u>
$CH_3Si_2$ ( $CH_3SiH_2SiH_3$ )	Methyl disilane	Ground state and Stark effect.
$C_7H_8O$ (  )	Bicyclo(2.2.1)hept-2-ene-5-one	Ground state and $V=3$ of lowest frequency vibration. Stark effect.
$C_7H_8O$ (  )	Tricyclo(2.2.1.0 <sup>2,6</sup> )heptanone	Ground state rotational constants.
$C_7H_{10}O$ (  )	Bicyclo(2.2.1)heptan-2-one	Ground state and $V=3$ of lowest frequency vibration. Stark effect.
$C_7H_{10}O$ (  )	Exo-3-oxatricyclo(3.2.1.0 <sup>2,4</sup> )-octane	Ground state rotational constants.
$C_8H_{12}O$ (  )	Bicyclo(2.2.2)octanone	Broad band assignment.
$C_{10}H_{14}O$ (  )	Tricyclo(3.3.1.1 <sup>3,7</sup> )decanone	Ground state rotational constants.

36. Sagami Chemical Research Center  
Sagamihara, Kanagawa 229, Japan

Yonezo MORINO

<u>Formula</u>	<u>Name of Compound</u>	<u>Name of Investigator</u>	<u>Present Stage of Progress</u>
HCO DCO	Formyl radical	S. Saito	Further work in progress.
C <sub>7</sub> H <sub>8</sub> S	endo- and exo-2,3-epithio-5-norbornene	F. Makino	Manuscript in preparation.



37. Name of Institution Institute of Physical and Chemical Research  
 Name of Department or Institute Microwave Physics Laboratory Wako-Shi, Saitama  
351 Japan  
 Name to Whom Queries Should Be Addressed Michio Takami

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH <sub>2</sub> O <sub>2</sub> (HCOOH)	Formic acid	Michio Takami	Seventeen lines in the $\nu_{CH}=1$ state observed and assigned.

38. Name of Institution: University of South Carolina  
 Name of Department or Institute: Department of Chemistry  
 Name to Whom Queries Should be Addressed: J. R. Durig

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STATE OF PROGRESS</u>
C <sub>2</sub> H <sub>10</sub> BP	dimethylphosphineborane	Hudgens	Spectra assigned for seven isotopic species

$C_4H_4F_4$	1,1,2,2-tetrafluorocyclobutane	Hudgens	Stark effect and excited states.
$C_2H_7P$	dimethylphosphine	Hudgens	Torsional barrier
$C_7H_{10}O$	bicyclo[2,2,1]heptane-7-one	Lopata	Draft
$C_7H_8O$	bicyclo[2,2,1]hept-2-ene-7-one	Li	Draft
$C_2H_8Ge$	ethylgermane	Lopata	Assigned
$CH_8BP$	methylphosphineborane	Kalasinsky	Excited states
$C_2H_7P$	ethylphosphine	Cox	Assigned
$C_4H_{12}N_2$	tetramethylhydrazine	Wurrey	In progress
$CH_3Cl_3Ge$	methyltrichlorogermane	MacNamee, Cooper	Assigned
$C_2D_3F_3$	methylfluoroform	Bucy	Excited states
$C_3H_8N_2$		Wilson	In progress
$C_2H_3ClO_2$	methylchloroformate	Griffin	Spectra assigned for seven isotopic species

39. Name of Institution: University of Southern California

Name of Department: Department of Chemistry

Name to Whom Queries should be addressed: Dr. Robert A. Beaudet

<u>Formula</u>	<u>Name of Compound</u>	<u>Name of Investigator</u>	<u>Present State of Progress</u>
$CB_5H_7$	Carbahexaborane (7)	B. Don	Submitted
$B_2H_8N(B_2H_8NH_z)$	Amino diborane	K. Lau	Submitted
$B_6H_{10}$	Hexaborane	K. Lau	Started
$C_2B_6H_8$	Dicarbaoctaborane (8)	K. Lau and H. Rogers	Manuscript in preparation
$C_2B_7H_9$	Dicarb nonaborane (9)	K. Lau	Assigned
$SiF_3SiH_3$	Trifluoro silane	Pasinski and McMahon	Manuscript in preparation



40. Name of Institution ..... University of Stockholm  
 Name of Department or Institute ..... Physical Chemistry  
 Name to Whom Queries Should Be Addressed ..... Fred Karlsson

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_4H_3Cl$	Chlorobutatriene	Fred Karlsson Ragnar Vestin Astrid Borg	Published
$C_4H_3Cl$	trans-1-Chlorobuten-3-yne	Fred Karlsson Ragnar Vestin	Published
$C_4H_3Cl$	cis-1-Chlorobuten-3-yne	Fred Karlsson Mats Granberg	Spectrum Observed
$C_4H_3Cl$	2-Chlorobuten-3-yne	Fred Karlsson Mats Granberg Ragnar Vestin	Published
$C_4H_3Cl$	4-Chlorobuten-3-yne	Fred Karlsson Mats Granberg	Substance Prepared

41. Name of Institution \_\_\_\_\_ Royal Institute of Technology, Fack, S-100 44 Stockholm 70, \_\_\_\_\_  
 Sweden.  
 Name of Department or Institute \_\_\_\_\_ Division of Physical Chemistry \_\_\_\_\_  
 Name to Whom Queries Should Be Addressed \_\_\_\_\_ Dr. Stig Ljunggren \_\_\_\_\_

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_6H_8O$	3-bicyclo(3.1.0)hexanone	J. Mjöberg	Ground state and five vibrational satellites assigned/

$C_8H_7F$	p-fluorostyrene	W. Ralowski	Ground state and seven vibrational satellites assigned.
$C_3H_6O_2S$	thietane dioxide	S. Ljunggren	Assignment in progress.
$C_4H_3BrS$	2-bromothiophene	J. Mjöberg	Work nearly completed.
$C_4H_3BrS$	3-bromothiophene	J. Mjöberg	Spectrum assigned.
$C_3H_4O_2S$	thietel, 1-dioxide	W. Ralowski	Manuscript submitted.

42. Name of Institution University of Sussex, Brighton, U.K.

Name of Department or Institute School of Molecular Sciences

Name to Whom Queries Should Be Addressed H. W. Kroto

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$CH_3NSi$ $SiH_3CN$	Silyl Cyanide	A. J. Careless	ms. prepared
$CH_3GeN$ $GeH_3CN$	Germy Cyanide	A. J. Careless	work suspended
$C_4H_9NSSi$ $(CH_3)_3SiNCS$	Trimethyl Silyl iso thio cyanate	A. J. Careless A. P. Cox	work still in progress
$C_2H_4S$ $CH_3CHS$	Thioacetaldehyde	B. Landsberg	$r_s$ structure complete barrier determined
$C_3H_6S$ $(CH_3)_2CS$	Thioacetone	B. Landsberg	barrier
$C_5H_{10}Si$ $(CH_3)_3SiCCH$	Trimethyl silyl acetylene	A. Alexander D. Walton	ground state spectrum assigned
$C_5H_4$ $CH_3CCCCH$	Methyl diacetylene	M. Maier	analysis of bending vib. satellites $v = 1-5$
$C_2H_2S$ $H_2CCS$	Thioketene	B. Landsberg K. Georgiou	structure and vib. satellites

43. SWISS FEDERAL INSTITUTE OF TECHNOLOGY

Laboratory for Physical Chemistry

Zurich, , Switzerland

Hs. H. Günthard / A. Bauder

$\text{CH}_3\text{NO}_2$	Nitromethane	A. Bauder	Internal rotation of deuterated species
$\text{C}_2\text{H}_4\text{O}$ ( $\text{CH}_3\text{COH}$ )	Acetaldehyde	A. Bauder	Structure relaxation
$\text{C}_3\text{H}_7\text{N}$ ( $\text{CH}_3\text{CH}=\text{NCH}_3$ )	N-Methylethylidenimine	W. Bossert	Deuterated species
$\text{C}_3\text{H}_4\text{O}_3$ ( $\text{CH}_3\text{COCO}_2\text{H}$ )	Pyruvic acid	Ch. Dyllik	Deuterated species
$\text{C}_2\text{H}_2\text{O}_2$ ( $\text{COH-COH}$ )	Glyoxal	M. Gut	IR/MW-double resonance and internal rotation
$\text{C}_2\text{H}_3\text{NO}_2$ ( $\text{CH}_2\text{CHNO}_2$ )	Nitroethylene	P. Nösberger	$^{15}\text{N}$ - and $^{18}\text{O}$ -species
$\text{O}_3+\text{CH}_2=\text{CH}_2$	Ozonides	S. Vaccani	Transient molecules

44. Name of Institution

Tata Institute of Fundamental Research  
Bombay, India

Name of Department or  
Institute

Chemical Physics Group

Name to Whom Queries  
should be Addressed

S.D. Sharma/S. Doraiswamy

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$\text{C}_6\text{F}_5\text{H}$	Pentafluorobenzene	S. Doraiswamy S.D. Sharma	In press (Pramana)
$\text{C}_5\text{F}_5\text{N}$	Pentafluoropyridine	S. Doraiswamy S.D. Sharma	In press (Chemical Physics)

$C_5H_4NCl$	3-Chloropyridine	S.D. Sharma S. Doraiswamy	Manuscript in preparation
$C_5H_4NF$	3-fluoropyridine	S. Doraiswamy S.D. Sharma	Analysis in progress
$C_5H_3F_2N$	2-6 difluoropyridine	S.D. Sharma S. Doraiswamy	Analysis in progress
$C_6F_4H_2$	2,4,5,6 fluorobenzene	S. Doraiswamy S.D. Sharma	Spectrum observed
$C_6F_5H_2$	2,3,4,5 fluorobenzene	S.D. Sharma S. Doraiswamy	Spectrum observed

45. Name of Institution Texas Tech University

Name of Department or Institute Department of Physics

Name to Whom Queries Should Be Addressed C. Richard Quade

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_6H_6S$ (normal and -SD and -CH <sub>2</sub> D species)	Ethyl mercaptan		<u>trans</u> and <u>gauche</u> spectra assigned; methyl internal rotation analysis for <u>trans</u> ; -SH and -SD internal rotation analysis in progress; partial two-top analysis.
$C_6H_6O$ (normal and -OD and -CH <sub>2</sub> D species)	Ethyl alcohol		substantial <u>gauche</u> spectra assigned; methyl internal rotation analysis for <u>gauche</u> ; -OH and -OD internal rotation analysis in progress; evidence of methyl-hydroxyl interaction.

$C_2H_3O_2N_3$  (normal and  $^{15}N$  Methyl-azido-formate Assignment and analysis nearly  
- $CD_3$  and  $^{15}N$  species) complete.

$C_7H_5OF$  meta-fluorobenzaldehyde cis and trans spectra assigned.

46. Name of Institution University of Texas at Austin  
Name of Department or Institute Department of Chemistry  
Name to Whom Queries Should Be Addressed Dr. James E. Boggs

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_8S$ ( $(CH_3)_2CHSH$ )	Isopropyl mercaptan	John Griffiths	Manuscript in preparation
$C_4H_5N$ ( $\underbrace{CH_2-CH_2-CH}_1-CN$ )	Cyclopropyl cyanide	R. E. Penn	Manuscript in preparation

47. Tokyo Institute of Technology  
Laboratory of Molecular Spectroscopy  
Professor Shiro Maeda

$C_2H_4S$ ( $CH_2SCH_2$ )	Ethylene sulfide	K. Okiye	$r_s$ ; Chem. Phys. Lett. <u>24</u> , 111, cooperation with Lister and Sheridan of Univ. of North Wales.
		K. Okiye	vib-rot interaction in progress.

$\text{CH}_3\text{I}$	Methyl iodide	Y. Kawashima	Fermi-Coriolis Bull. Chem. Soc. Japan, <u>46</u> , 2969.
$\text{CF}_3\text{D}$	Fluoroform	Y. Kawashima	Fermi-Coriolis analysis in progress.
$\text{C}_6\text{H}_5\text{NO}$ ( ) N CHO	2-Pyridine aldehyde	Y. Kawashima	trans-isomer, 5 vibl. states, manuscript.
$\text{C}_3\text{H}_5\text{NO}_2$ ( $\text{CH}_3\text{CH}_2\text{CHNO}_2$ )	trans-1-nitropropene	K. Tochigi	internal rot. and eQq(N), manuscript.
$\text{C}_2\text{H}_4\text{O}$ ( $\text{H}_2\text{C}_0\text{CH}_2$ )	Ethylene oxide	N. Yoshimizu	vib-rot interaction manuscript in prepn.
		C. Hirose	ten isotopes, $r_0$ , $r_s$ , $r_m$ ; Bull. Chem. Soc. Japan, accepted.
		C. Hirose	mm wave, Ap. J. Lett. in press.
$\text{C}_4\text{H}_6\text{O}$ (( $\text{CH}_2\text{CH}$ ) $_2\text{O}$ )	Divinyl ether	C. Hirose	vibrational states analysis in progress.

48. Name of Institution National Chemical Laboratory for Industry  
 Name of Department or Institute 2nd Division  
 Name to Whom Queries Should Be Addressed Chi Matsumura

Honmachi-1, Shibuya-ku, Tokyo

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$\text{C}_3\text{H}_6\text{F}_2$	2,2-Difluoropropane	Takeo	Normal, $d_1$ , $d_6$ , and $^{13}\text{C}$ species assigned Excited states in progress.

$\text{CCl}_2\text{F}_2$	Dichlorodifluoromethane	Takeo	Spectrum assigned
$\text{C}_2\text{H}_2\text{Cl}_2$	1,2-Dichloroethylene	Takeo	$r_s$ structure and $\chi$ 's determined
$\text{CH}_3\text{BF}_2\text{O} (\text{BF}_2\text{OCH}_3)$	Methoxy difluoroborane	Takeo	Work temporarily abandoned
$\text{C}_3\text{H}_6\text{Cl}_2$	2,2-Dichloropropane	Matsumura	Normal species assigned, $d_6$ in progress
$\text{C}_2\text{H}_4\text{Cl}_2$	1,2-Dichloroethane	Matsumura	$d_4$ species assigned

49. UNIVERSITY COLLEGE LONDON

Department of Chemistry

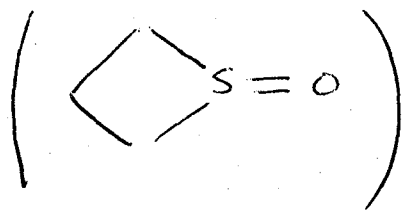
London, England

D. J. Millen/A. C. Legon

Trimethylene sulphoxide

J. W. Bevan

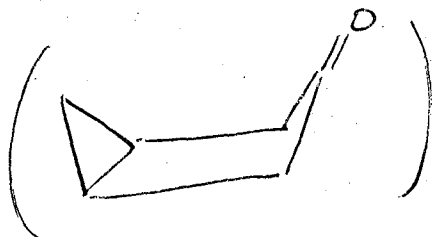
Manuscript in preparation



Bicyclo-[3-1-0] hexanone

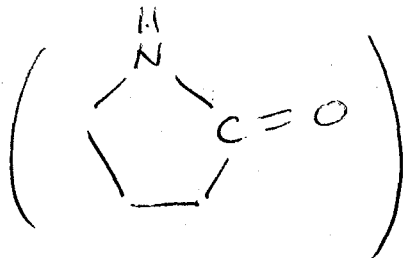
J. W. Bevan

Isotopic work in progress



Pyrrolidone

J. W. Bevan Isotopic work in progress



50 Name of Institution University of Ulm, D-79 Ulm, Germany

Name of Department or Institute Institute of Physical Chemistry

Name to Whom Queries Should Be Addressed H. D. Rudolph

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_2H_3N (CH_3NC)$	methyl isocyanide	M.Römheld in collaboration with T.Oka, NRC, Ottawa	partial assignment of laser-Stark spectrum, IR/MW-DR in progress
$C_2H_3NS (CD_3SCN)$	$d_3$ -methylthiocyanate	H.Schleser	PAM-, IAM-studies of 2 exc.tors. states completed
$C_2H_6S ((CD_3)_2S)$	$d_6$ -dimethylsulfide	B.T. Tan	01,10 exc.tors. states, paper in preparation
$C_2H_7SiCl$ $(CH_3CH_2SiH_2Cl)$	ethylchlorosilane	V. Typke in collaboration with W. Zeil, Tübingen	r-structure of trans-, gauche forms, paper in preparation



$C_3H_7N$ ( $CH_2CHCH_2NH_2$ )	allylamine	I. Botskor, H.D. Rudolph in collaboration with G.Roussy, Nancy	N-gauche, N-lone-pair- gauche form, paper accepted; N-gauche, N-lone-pair- trans form, paper submit- ted
$C_4H_2N_2$ ( $H_2CC(CN)_2$ )	vinylidenedicyanide	B.T. Tan J. Demaison	g. s., vibr. sat. assigned
$C_4H_8$ (( $CH_3$ ) $CCH_2$ )	isobutene	J. Demaison	01,10 exc.tors. states, paper accepted
$C_7H_7F$ ( $CH_2DC_6H_4F$ , $CHD_2C_6H_4F$ )	$\alpha d_1^-$ , $\alpha d_2^-$ ortho fluorotoluene	D. Schwach	g. s. asymm. int. rotor studies com- pleted, paper in preparation
$C_7H_7F$ ( $CH_2DC_6H_4F$ , $CHD_2C_6H_4F$ )	$\alpha d_1^-$ , $\alpha d_2^-$ para fluorotoluene	H. Schleser	exc. state asymm. int. rotor studies concluded
$C_7H_8$ ( $CH_2DC_6H_5$ )	$d_1$ -toluene	H. Schleser	exc. state asymm. int. rotor studies concluded
$H_3N$	ammonia	H. Jones W.A. Kreiner	IR/MW double and triple resonance study of hfs, paper accep- ted
$H_3N$	ammonia	H. Jones W.A. Kreiner A. Eyer	collisional transfer by IR/MW-DR, paper submit- ted

51. Name of Institution Rijksuniversiteit Utrecht, The Netherlands  
 Name of Department or Institute Fysisch Laboratorium  
 Name to Whom Queries Should Be Addressed B.P. van Eijck / H.A. Dijkerman

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_2H_3ClO_2$ ( $CH_2ClCOOH$ )	Chloroacetic acid	van Eijck	In press
$CH_3ClO_2S$ ( $SO_2ClCH_3$ )	Methane sulfonyl chloride	van Eijck	Paper submitted
$C_2H_2F_2O_2$ ( $CHF_2COOH$ )	Difluoroacetic acid	Bijen	In progress
$C_2HF_3O_2$ ( $CF_3COOH$ )	Trifluoroacetic acid	Maagdenberg	In progress

52. Name of Institution Virginia Polytechnic Institute and State University  
 Name of Department or Institute Chemistry  
 Name to Whom Queries Should Be Addressed Jack D. Graybeal

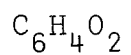
<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_2H_2BrN(CH_2BrCN)$	Monobromoacetonitrile	M.L.Gum	Spectrum assigned, deuterated species in progress, manuscript in prep.
$F_4OS(F_4SO)$	Sulfur oxytetrafluoride	C.Shoemaker M.L.Gum	spectrum assigned, manuscript in prep
$CrF_2O_2$	Chromyl fluoride	C.Shoemaker	work in progress

53. Name of Institution University of Wisconsin  
 Name of Department or Institute Chemistry  
 Name to Whom Queries Should Be Addressed R. Claude Woods

<u>FORMULA*</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR**</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>10</sub> O	(C(CH <sub>3</sub> ) <sub>3</sub> OH) t-butyl alcohol	E. Valenzuela	in progress
C <sub>4</sub> H <sub>10</sub> S	(C(CH <sub>3</sub> ) <sub>3</sub> SH) t-butyl mercaptan	E. Valenzuela	work completed
C <sub>6</sub> H <sub>8</sub>	(CH <sub>2</sub> CCH <sub>2</sub> CH <sub>2</sub> C CH <sub>2</sub> ) dimethylene cyclobutane	R. Saykally	in progress

54. Name of Institution: MONASH UNIVERSITY  
 Name of Department : CHEMISTRY DEPARTMENT  
 Name to Whom Queries should be addressed: PROFESSOR R.D. BROWN

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STATE OF PROGRESS</u>
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	pyrimidine	E. Clarke	paper in preparation
C <sub>2</sub> H <sub>3</sub> NO <sub>3</sub>	peroxyacetylnitrate (PAN)	M. Haynes P. Sinclair	work continuing
C <sub>5</sub> H <sub>4</sub> NCl	m-chloropyridine	J. Matouskova	spectrum assigned N.Q.R. analysis complete.
C <sub>6</sub> H <sub>6</sub>	dimethylenecyclobutene	A. Ottrey	work continuing



o-benzoquinone

A. Porter

work in progress



hydrogen isocyanide

H. Gunn

work in progress



dewar benzene

D. Griffith

accepted for  
publication  
Chem. Phys. Letts.



UNIVERSIDAD DE BUENOS AIRES  
FACULTAD DE CIENCIAS EXACTAS Y NATURALES

Name of Institution: Facultad de Ciencias Exactas, Universidad de Buenos Aires.  
Name of Department: Departamento de Física.  
Name to Whom Queries Should Be Addressed: Lic. T. Hartmann.

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STATE OF PROGRESS
$C_6F_4H_2$	1,2,3,4 Tetrafluorebenzene.	T. Hartmann.	Work continued on centrifugal distertion.
$C_6F_4H_2$	1,2,3,5 "	{ T. Hartmann. I. Botsker.	Work started.
$C_6F_3H_3$	1,2,4 Trifluorebenzene.	{ T. Hartmann. A. Galván.	Work started.
$CH_2=CHCH_2CH$	Allyleyanide.	{ T. Hartmann. I. Botsker.	Excited states.
$C_2O_2Cl_2$	Oxalyl Chleride.	M. López Iglesias.	Work started.

FORMULA INDEX

- AB - Diatomic molecules - 24
- AlF - Aluminum monofluoride - 2/3
- BF<sub>3</sub>Si - (SiF<sub>3</sub>BF<sub>2</sub>) - difluoro(trifluorosilyl) borane - 3
- B<sub>2</sub>H<sub>8</sub>N - (B<sub>2</sub>H<sub>8</sub>NH<sub>2</sub>) - Amino diborane - 39
- B<sub>6</sub>H<sub>10</sub> - Hexaborane - 39
- BaO - Barium oxide - 2/3
- BaS - Barium sulfide - 2/3
- BrCl - Bromine chloride - 2/3
- BrCs - (CsBr) - Cesium bromide - 2/3
- BrF<sub>3</sub>Si - (SiF<sub>3</sub>Br) - trifluorosilyl bromide - 3
- BrF<sub>5</sub> - Bromine pentafluoride - 15
- BrI - (IBr) - Iodine bromide - 2
- BrIn - (InBr) - Indium bromide - 2
- BrRb - (RbBr) - Rubidium bromide - 2
- CB<sub>2</sub>O - (OCBr<sub>2</sub>) - Carbonyl bromide - 27
- CB<sub>2</sub>S - (SCBr<sub>2</sub>) - Thiocarbonyl bromide - 27
- CClFO - Carbonylfluorochloride - 13
- CCl<sub>2</sub>F<sub>2</sub> - Dichlorodifluoromethane - 48
- CCl<sub>2</sub>S - (SCCl<sub>2</sub>) - Thiocarbonyl chloride - 27
- CF<sub>3</sub>NO<sub>2</sub> - Trifluoronitromethane - 3
- CN<sub>2</sub>O - (NO.CN) - Nitrosyl cyanide - 9
- COS - (OCS) - Carbonyl sulphide - 17, 24
- COS - <sup>16</sup>O<sup>12</sup>C<sup>32</sup>S - <sup>16</sup>O<sup>13</sup>C<sup>32</sup>S - 7
- CF<sub>3</sub>D - Fluoroform - 47
- CHNO (HCNO, DCNO) Fulminic acid - 8
- CHNO - (HNCO) - Isocyanic acid, all isotopic species - 8
- CHO - (HCO, DCO) - Formyl radical - 36
- CH<sub>2</sub>F<sub>2</sub> - CD<sub>2</sub>F<sub>2</sub> - Methylene fluoride - 14
- CH<sub>2</sub>O<sub>2</sub> - (HCOOH) - Formic acid - 37
- CH<sub>3</sub>BF<sub>2</sub> - Methyl boron difluoride - 13
- CH<sub>3</sub>BF<sub>2</sub>O - (BF<sub>2</sub>OCH<sub>3</sub>) - Methoxy difluoroborane - 48
- CH<sub>3</sub>Br - Methyl bromide - 17
- CH<sub>3</sub>Cl - (CHD<sub>2</sub><sup>35</sup>Cl) - (CHD<sub>2</sub><sup>37</sup>Cl) - Methyl chloride - 33
- CH<sub>3</sub>Cl - (CD<sub>3</sub>Cl) - Methyl chloride - 14
- CH<sub>3</sub>ClO<sub>2</sub>S - (SO<sub>2</sub>ClCH<sub>3</sub>) - Methane sulfonyl chloride - 51
- CH<sub>3</sub>ClS - (CH<sub>3</sub>SCL) - Methane sulfenyl chloride - 13
- CH<sub>3</sub>Cl<sub>3</sub>Ge - Methyltrichlorogermane - 38
- CH<sub>3</sub>F - (CD<sub>3</sub>F) - Methyl fluoride - 14
- CH<sub>3</sub>F<sub>2</sub>P - (CH<sub>3</sub>PF<sub>2</sub>) - Methyl difluorophosphine - 19
- CH<sub>3</sub>F<sub>3</sub>Ge - (CF<sub>3</sub>GeH<sub>3</sub>) - Trifluoromethyl-germane - 16
- CH<sub>3</sub>GeN - (GeH<sub>3</sub>CN) - Germyl cyanide - 42
- CH<sub>3</sub>HgX - (X=Cl, Br, I) - Methyl mercury derivatives - 1
- CH<sub>3</sub>I - (CH<sub>2</sub>DI) - Methyl iodide - 33

- $\text{CH}_3\text{I}$  - Methyl iodide - 47  
 $\text{CH}_3\text{NO}$  - Nitrosomethane - 3  
 $\text{CH}_3\text{NO}$  - ( $\text{HCONH}_2$ ) - Formamide, -CD, -NHD, -ND,  $^{-15}\text{N}, ^{-13}\text{C}, ^{-18}\text{O}$  - 7  
 $\text{CH}_3^{15}\text{NO}$  - ( $\text{CHO}^{15}\text{NH}_2$ ) -  $^{15}\text{N}$ -formamide - 8  
 $\text{CH}_3\text{NO}_2$  - Nitromethane - 33, 13, 43  
 $\text{CH}_3\text{NSi}$  - ( $\text{SiH}_3\text{CN}$ ) - Silyl cyanide - 42  
 $\text{CH}_4$  - ( $\text{CH}_2\text{D}_2$ ) - Methane - 14  
 $\text{CH}_4\text{O}$  - ( $\text{CH}_3\text{OH}$ ) - Methyl alcohol - 17  
 $\text{CH}_5\text{As}$  - ( $\text{CH}_3\text{AsH}_2$ ) - Methyl arsine - 29  
 $\text{CH}_5\text{FGe}$  - ( $\text{CH}_2\text{FGeH}_3$ ) - Fluoromethyl-germane - 16  
 $\text{CH}_5\text{NO}$  - ( $\text{CH}_3\text{ONH}_2$ ) - Methoxyamine - 12  
 $\text{CH}_6\text{BF}_2\text{P}$  - ( $\text{CH}_3\text{PF}_2\text{BH}_3$ ) - Methyl difluoro-phosphine- $\text{BH}_3$  - 19  
 $\text{CH}_6\text{OSi}$  - ( $\text{CH}_3\text{OSiH}_3$ ) - Silyl methyl ether - 34  
 $\text{CH}_7\text{B}_5$  - Carbahexaborane (7) - 39  
 $\text{CH}_8\text{BP}$  - ( $\text{CH}_3\text{PH}_2\text{BH}_3$ ) - Methyl phosphine-borane - 38  
 $\text{CH}_8\text{Si}_2$  - ( $\text{CH}_3\text{SiH}_2\text{SiH}_3$ ) - Methyl disilane - 35  
 $\text{C}_2\text{HF}_3\text{O}_2$  - ( $\text{CF}_3\text{COOH}$ ) - Trifluoroacetic acid - 51  
 $\text{C}_2\text{H}_2\text{BrN}$  - ( $\text{CH}_2\text{BrCN}$ ) - Monobromoacetonitrile - 52  
 $\text{C}_2\text{H}_2\text{ClFO}$  - Fluoroacetyl chloride - 18  
 $\text{C}_2\text{H}_2\text{Cl}_2$  - 1,2-Dichloroethylene - 48  
 $\text{C}_2\text{H}_2\text{F}_2\text{O}_2$  - ( $\text{CHF}_2\text{COOH}$ ) - Difluoroacetic acid - 51  
 $\text{C}_2\text{H}_2\text{F}_2\text{O}_3$  - ( $\text{HFCOOCHF}_2$ ) - cis- and trans- 1,2-difluoroethylene ozonide - 11  
 $\text{C}_2\text{H}_2\text{F}_2\text{O}_3$  - ( $\text{F}_2\text{COOCH}_2\text{O}$ ) - 1,1-difluoroethylene ozonide - 11  
 $\text{C}_2\text{HDO}$  - ( $\text{HDCCO}$ ) - Monodeuteroketene - 8  
 $\text{C}_2\text{H}_2\text{O}$  - ( $\text{D}_2\text{CCO}$ ) - Dideuteroketene - 8, 13  
 $\text{C}_2\text{H}_2\text{O}_2$  - ( $\text{COH-COH}$ ) - Glyoxal - 43  
 $\text{C}_2\text{H}_2\text{O}_3$  - ( $\text{CHOCOOH}$ ) - Glyoxylic acid - 28  
 $\text{C}_2\text{H}_2\text{S}$  - ( $\text{H}_2\text{CCS}$ ) - Thioketene - 42  
 $\text{C}_2\text{H}_3\text{ClO}$  - Chloroacetaldehyde - 18  
 $\text{C}_2\text{H}_3\text{ClO}_2$  - ( $\text{CH}_2\text{ClCOOH}$ ) - Chloroacetic acid - 51  
 $\text{C}_2\text{H}_3\text{ClO}_2$  - Methylchloroformate - 38  
 $\text{C}_2\text{H}_3\text{FO}_3$  - ( $\text{FH COOCH}_2\text{O}$ ) - 1-fluoroethylene ozonide - 20  
 $\text{C}_2\text{D}_3\text{F}_3$  - Methylfluoroform - 38  
 $\text{C}_2\text{H}_3\text{N}$  - ( $\text{CH}_3\text{CN}$ ) - Methyl cyanide  $\text{CHD}_2\text{CN}$  - 33  
 $\text{C}_2\text{H}_3\text{NO}$  - ( $\text{CH}_3\text{CNO}$ ) - Methylfulmide - 8  
 $\text{C}_2\text{H}_3\text{NO}_2$  - ( $\text{CH}_2\text{CHNO}_2$ ) - Nitroethylene - 43  
 $\text{C}_2\text{H}_3\text{NO}_3$  - (PAN) - peroxyacetylnitrate - 54  
 $\text{C}_2\text{H}_3\text{NS}$  - ( $\text{CD}_3\text{SCN}$ ) -  $d_3$ -Methylthiocyanate - 50  
 $\text{C}_2\text{H}_3\text{N}_3$  - 1,2,3-triazole 1-D species - 7  
 $\text{C}_2\text{H}_3\text{N}_3\text{O}_2$  - ( $\text{CH}_3\text{OCON}_3$ ) - Methyl-azido-formate (normal and - $\text{CD}_3$  and  $^{15}\text{N}$  species) - 45  
 $\text{C}_2\text{H}_3\text{SN}$  - ( $\text{CH}_3\text{SCN}$ ) - Methyl thiocyanate - 13  
 $\text{C}_2\text{H}_4\text{Cl}_2$  - 1,2-Dichloroethane - 48  
 $\text{C}_2\text{H}_4\text{FNO}$  - ( $\text{CH}_2\text{FCONH}_2$ ) - 2-Fluoroacetamide - 28  
 $\text{C}_2\text{H}_4\text{O}$  - Acetaldehyde - 43  
 $\text{C}_2\text{H}_4\text{O}$  - ( $\text{CH}_2\text{CH}_2\text{O}$ ) - Ethylene oxide - 19, 47  
 $\text{C}_2\text{H}_4\text{OS}$  - ( $\text{HCO.SCH}_3$ ) - Methyl thiolformate - 1  
 $\text{C}_2\text{H}_4\text{O}_3$  - ( $\text{H}_2\text{COOCH}_2\text{O}$ ) - Ethylene ozonide - 20  
 $\text{C}_2\text{H}_4\text{S}$  - ( $\text{CH}_3\text{CHS}$ ) - Thioacetaldehyde - 42  
 $\text{C}_2\text{H}_4\text{S}$  - ( $\text{CH}_2\text{SCH}_2$ ) - Ethylene sulfide - 47

$C_2H_5ClO$ - Chloromethyl Methyl Ether - 10, 34	$C_3H_2N_2$ - $[CH_2(CN)_2]$ - Methylene cyanide (malononitrile) - 21
$C_2H_5N$ - $(CH_3CH=NH)$ - <u>cis</u> -C-Methyl methyleneimine - 24	$C_3H_3FO$ - Acryloyl fluoride - 34
$C_2H_5N$ - $(CH_3CH=NH)$ - <u>trans</u> -C-Methyl methyleneimine - 24	$C_3H_3F_3O_2$ - $(CF_3COOCH_3)$ - Methyl trifluoro- methylacetate - 6
$C_2H_5N$ - $(CH_2=CHNH)$ - Vinylamine - 24	$C_3H_3N$ - $(CH_3NC)$ - Methyl isocyanide - 50
$C_2H_5NO$ - $(CH_3CONH_2)$ - Acetamide - 11	$C_3H_3N$ - $(CH_2CHNC)$ - Vinyl isocyanide - 8
$C_2H_5NO$ - $(HCONHCH_3)$ - N-Methylformamide - 19	$C_3H_3NO$ - Isoxazole - 1
$C_2H_6F_3NSi$ - $(SiF_3N(CH_3)_2)$ - Trifluorosilyl- dimethylamine - 3	$C_3H_4$ - Cyclopropene - 30
$C_2H_6N_2O$ - $[(CH_3)_2NNO]$ - Dimethylnitrosamine - 13	$C_3H_4ClN$ - $(ClCH_2CH_2CN)$ - 3 Chloropropio- nitrile - 11
$C_2H_6N_2O_2$ - $[(CH_3)_2NNO_2]$ - dimethylnitramine - 13	$C_3H_4Cl_2F_2O$ - $(CHCl_2CF_2-O-CH_3)$ 2,2-dichloro- 1,1-difluoroethyl methyl ether -
$C_2H_6O_2$ - $(CH_2OHCH_2OH)$ - Ethylene glycol - 28	$C_3H_4F_2$ - 3,3-Difluoropropene - 14
$C_2H_6S$ - $[(CD_3)_2S]$ - $d_6$ -Dimethylsulfide - 50	$C_3H_4F_2$ - 1,1-Difluorocyclopropane - 30
$C_2H_6S_2$ - $(HSCH_2-CH_2SH)$ - 1,2-Ethanedithiol - 11	$C_3H_4F_2O$ - $(CH_2FCOCH_2F)$ 1,3-difluoroacetone -10, 11
$C_2H_6S_2$ - $(CD_3SSCH_3)$ - Trideuteromethyl-methyl disulfide - 13	$C_3H_4Hg$ - $(CH_3HgCCH)$ - 1
$C_2H_7As$ - $[(CH_3)_2AsH]$ - Dimethylarsine - 29	$C_3H_4N_2$ - Pyrazole - 7
$C_2H_7ClSi$ - $(CH_3CH_2SiH_2Cl)$ - Ethylchloro- silane - 50	$C_3H_4N_2$ - Imidazole - 1
$C_2H_7N$ - Ethylamine - 30	$C_3H_4O$ - $(CH_2CHCHO)$ - Acrolein - 8, 14
$C_2H_7P$ - Dimethylphosphine - 38	$C_3H_4OS$ - Thietanone-3 - 21
$C_2H_7P$ - Ethylphosphine - 38	$C_3H_4O_2$ - $(CH_2OCHCHO)$ - Glycidaldehyde - 19
$C_2H_8B_6$ - Dicarbaoctaborane (8) - 39	$C_3H_4O_2$ - $(O=CH-CH=CH-OH)$ - Malondialdehyde - 1
$C_2H_8Ge$ - Ethyl germane - 38	$C_3H_4O_2S$ - Thietel, 1-dioxide - 41
$C_2H_9B_7$ - Dicarba nonaborane (9) - 39	$C_3H_4O_3$ - $(CH_3COCOOH)$ - Pyruvic acid - 43
$C_2H_{10}BP$ - Dimethyl phosphineborane - 38	$C_3H_5N$ - $(CH_3CH_2CN)$ - Propionitrile - 13
$C_3H_2F_4$ - Tetrafluorocyclopropane - 30	



- $C_3H_5NO$  - Methoxyacetonitrile - 28, 32  
 $C_3H_5NO_2$  -  $(CH_3CH_2CHNO_2)$  - trans-1-nitropropene - 47  
 $C_3H_5FO$  -  $(CH_2FC(=O)CH_3)$  - Fluoroacetone - 13  
 $C_3H_6Cl_2$  - 2,2-Dichloropropane - 48  
 $C_3H_6F_2$  - 2,2-Difluoropropane - 48  
 $C_3H_6O$  -  $(C_3H_5OH, OD)$  - Cyclopropanol - 1  
 $C_3H_6O$  - Oxetane- $\alpha_2$  - 33  
 $C_3H_6O$  -  $(CH_3CH_2CHO)$  - Propanal - 11  
 $C_3H_6OS$  - Trimethylene sulphoxide - 49  
 $C_3H_6O_2$  -  $(CH_2-O-CH-CH_2OH)$  - Glycidol - 25  
 $C_3H_6O_2$  -  $(CH_3CH_2CO_2H)$  - Propionic acid - 1  
 $C_3H_6O_2S$  - Thietane dioxide - 41  
 $C_3H_6S$  -  $[(CH_3)_2CS]$  - Thioacetone - 42  
 $C_3H_7ClO$  -  $(ClCH_2CH_2CH_2OH)$  - Chloropropanol - 11  
 $C_3H_7N$  -  $(CH_2=CHCH_2NH_2)$  - Allylamine - 23, 50  
 $C_3H_7N$  - Cyclopropylamine - 12  
 $C_3H_7N$  -  $(CH_3CH=NCH_3)$  - N-Methylethylidenimine - 43  
 $C_3H_7NO$  -  $[HCON(CH_3)_2]$  - Dimethylformamide - 19  
 $C_3H_8N_2$  - 38  
 $C_3H_8O, C_3H_7OD$  -  $[(CH_3)_2CHOH, (CH_3)_2CHOD]$  - Isopropanol - 14  
 $C_3H_8S$  -  $[(CH_3)_2CHSH]$  - Isopropyl mercaptan - 46  
 $C_3H_9NO$  - 3-Amino propanol - 34  
 $C_3H_9NO$  - 2-Methylaminoethanol - 22  
 $C_3H_{12}BN$  -  $[(CH_3)_3NBH_3]$  - Trimethylamine borane - 20  
 $C_4H_2N_2$  -  $[H_2CC(CN)_2]$  - Vinylidenedicyanide - 50  
 $C_4H_3BrS$  - 2-Bromothiophene - 41  
 $C_4H_3BrS$  - 3-Bromothiophene - 41  
 $C_4H_3Cl$  - Chlorobutatriene - 40  
 $C_4H_3Cl$  - 2-Chlorobuten-3-yne - 40  
 $C_4H_3Cl$  - 4-Chlorobuten-3-yne - 40  
 $C_4H_3Cl$  - cis-1-Chlorobuten-3-yne - 40  
 $C_4H_3Cl$  - trans-1-Chlorobuten-3-yne - 40  
 $C_4H_4F_4$  - 1,1,2,2-Tetrafluorocyclobutane - 38  
 $C_4H_4N_2$  - Pyrimidine - 54  
 $C_4H_4O_2$  -  $(HCO.OCH_2CCH)$  - Propargyl formate - 1  
 $C_4H_5F_3O$  -  $(CF_3CH_2-O-CH=CH_2)$  - 2,2,2-Trifluoroethyl vinyl ether - 6  
 $C_4H_5F_3O_2$  -  $(CF_3COOC_2H_5)$  - Ethyl trifluoromethyl acetate - 6  
 $C_4H_5N$  - Cyclopropyl cyanide - 22, 30, 46  
 $C_4H_5NS$  -  $(CH_2=CHCH_2NCS)$  - Allylisothiocyanate - 23  
 $C_4H_6O$  - Butadiene monoxide - 34  
 $C_4H_6O$  - 3-Butyn-1-ol - 18  
 $C_4H_6O$  -  $[(CH_2CH)_2O]$  - Divinyl ether - 47  
 $C_4H_6O_2$  - 2,3-Dihydro-p-dioxin (1,4-dioxene) - 2  
 $C_4H_7Cl$  -  $[CH_2C(CH_3)CH_2Cl]$  - Isobutenyl chloride - 11  
 $C_4H_7N$  -  $(CH_3CH_2CH_2NC)$  - n-Propyl isocyanide - 1  
 $C_4H_7NO$  - Pyrrolidone - 49  
 $C_4H_7NO$  -  $[Me_2C(OH)CN]$  - Acetone cyanohydrin - 1

- $C_4H_7OX$  -  $(Me_2CHCOX)$  ( $X=H,F,OH$ ) - Isobutyric aldehyde, acid, acid fluoride - 1  
 $C_4H_8$  -  $[(CH_3)CCH_2]$  - Isobutene - 50  
 $C_4H_8O$  -  $(CH_3CH_2CH_2CHO)$  - n-Butyraldehyde - 19  
 $C_4H_8O$  -  $(C_4H_7OH,OD)$  - Cyclobutanol - 1  
 $C_4H_8O$  - 1-Me-cyclopropanol - 1  
 $C_4H_8OS$  - 1,4-Thioxane - 21  
 $C_4H_8O_2$  - 1,3-Dioxane - 32  
 $C_4H_8O_3$  -  $(CH_3CHOOCHCH_3O)$  - cis-2-butene ozonide - 11  
 $C_4H_9NSSi$  -  $[(CH_3)_3SiNCS]$  - Trimethyl Silyl iso thio cyanate - 42  
 $C_4H_{10}O$  -  $[C(CH_3)_3OH]$  - t-Butyl alcohol - 53  
 $C_4H_{10}S$  -  $[C(CH_3)_3SH]$  - t-Butyl mercaptan - 53  
 $C_4H_{11}NO$  - 2-Dimethylaminoethanol - 22  
 $C_4H_{12}N_2$  - Tetramethylhydrazine - 38  
 $C_5F_5N$  - Pentafluoropyridine - 44  
 $C_5H_3F_2N$  - 2-6 Difluoropyridine - 44  
 $C_5H_4$  -  $(CH_3CCCCH)$  - Methyl diacetylene - 42  
 $C_5H_4$  - 1,4 Pentadiyne - 20  
 $C_5H_4ClN$  - 2-Chloropyridine - 21  
 $C_5H_4NCl$  - 3-Chloropyridine - 44, 54  
 $C_5H_4NF$  - 3-Fluoropyridine - 44  
 $C_5H_4N_2$  - 1,1-Dicyanocyclopropane - 30  
 $C_5H_5As$  - Arsabenzene - 20  
 $C_5H_5N$  - Pyridine - 7  
 $C_5H_5NNiO$  -  $[C_5H_5NiNO]$  - Cyclopentadienyl nickel nitrosyl - 3  
 $C_5H_5NO$  - Pyridine N-oxide - 7  
 $C_5H_5NO$  - Pyrrole-2-carboxaldehyde - 28  
 $C_5H_5Tl$  - Cyclopentadienyl thallium - 3  
 $C_5H_6$  - 1,2,4-Pentatriene (vinylallene) - 7  
 $C_5H_6N_2$  - 3-Aminopyridine - 1  
 $C_5H_6N_2$  - 4-Aminopyridine - 1  
 $C_5H_6O$  - 3-Methylfuran - 13  
 $C_5H_6O$  - Oxaspiropentane - 4  
 $C_5H_7F_3O_2$  -  $(CF_3COOCH_2CH_2CH_3)$  - n-Propyl trifluoromethyl acetate - 6  
 $C_5H_7F_3O_2$  -  $[CF_3COOCH(CH_3)_2]$  - Isopropyl trifluoromethyl acetate - 6  
 $C_5H_8$  - 1,2-Pentadiene - 18  
 $C_5H_8$  -  $[CH_2=CHCH_2CH=CH_2]$  - 1,4-Pentadiene 14  
 $C_5H_8O$  - Cyclopent-3-ene-1-ol - 1  
 $C_5H_8O$  - 3,6-Dihydro-2H-pyran - 21  
 $C_5H_8O$  - 1-Methoxybutadiene - 32  
 $C_5H_8O$  -  $[Me_2C(OH)CCH]$  - 2-Methyl-3-butyn-2-ol - 1  
 $C_5H_8O$  - 3-Oxabicyclo(3.1.0.)hexane - 21  
 $C_5H_{10}N_2$  - Tert-butyl cyanamide - 32  
 $C_5H_{10}O$  - 3,3-Dimethyl oxetane - 33  
 $C_5H_{10}O$  - Tetrahydropyran - 32  
 $C_5H_{10}Si$  -  $[(CH_3)_3SiCCH]$  - Trimethyl silyl acetylene - 32  
 $C_5H_{11}N$  - Piperidine (axial NH) - 32  
 $C_5H_{11}NO$  - N-methyl morpholine - 32  
 $C_6HF_6$  - Pentafluorobenzene - 44

$C_6H_2F_4$ - 2,3,4,5 Fluorobenzene - 44	$C_6H_8$ - Bicyclo[2.1.1]hex-2-ene - 12
$C_6H_2F_4$ - 2,4,5,6 Fluorobenzene - 44	$C_6H_8$ - $(CH_2CCH_2CH_2C, CH_2)$ - Dimethylene cyclo- butane - 53
$C_6H_2F_4$ 1-2-3-4 Tetrafluorobenzene - 26	$C_6H_8$ - 1,2-Dimethylenecyclo-butane - 21
$C_6H_4F_2$ - 1,3-Difluorobenzene - 13	$C_6H_8$ - Tricyclo(2.2.0.0 <sup>2,6</sup> )hexane - 11
$C_6H_4N_2$ - 3-Cyanopyridine - 18	$C_6H_8O$ - Bicyclo-[3-1-0]hexanone - 49
$C_6H_4N_2$ - 4-Cyanopyridine - 18	$C_6H_8O$ - 3-Bicyclo(3.1.0)hexanone - 41
$C_6H_4O_2$ - o-Benzoguinone - 54	$C_6H_{10}$ - Bicyclo(3.1.0.)hexane - 21
$C_6H_5BF_2$ - Phenyl boron difluoride - 1	$C_6H_{10}$ - 2-Methyl bicyclo[2.1.0]pentane - 12
$C_6H_5BrO$ - 4-Br-phenol - 7	$C_6H_{10}S$ - 7-Thiabicyclo[2.2.1]heptane - 14
$C_6H_5Cl$ - Chlorobenzene - 23	$C_6H_{12}O$ - Oxepane - 32
$C_6H_5ClO$ - 4-C -phenol - 7	$C_6H_{12}Si$ - 1-Silabicyclo[2.2.1]heptane - 14
$C_6H_5FO$ - 4-F-phenol - 7	$C_6H_{13}N$ - N-methyl piperidine - 32
$C_6H_5FS$ - 4-F-thiophenol-SD - 7	$C_7H_5F_3$ - $(C_6H_5CF_3)$ - Benzotrifluoride - 3
$C_6H_5NO$ - 2-Pyridine aldehyde - 47	$C_7H_5N$ - Phenylisocyanide - 7
$C_6H_5NO_2$ - Nitrobenzene - 7	$C_7H_5NO$ - $(C_6H_5NCO)$ - Phenyliso-cyanate - 23
$C_6H_6$ - Dimethylenecyclobutene, dewar benzene- $C_6H_6FN$ - o-Fluoroaniline - 1 54	$C_7H_5NS$ - $(C_6H_5NCS)$ - Phenylisothio-cyanate - 23
$C_6H_6O$ - Ethyl Alcohol - (normal and -OD and -CH <sub>2</sub> D species) - 45	$C_7H_5OF$ - Meta-fluorobenzaldehyde - 45
$C_6H_6O$ - Phenol-OD, phenol, phenol-OD, phenol- <sup>13</sup> C - 7	$C_7H_7F$ - $(CH_2DC_6H_4F)$ - $\alpha_{d_1}$ -Orthofluorotoluene - 50
$C_6H_6S$ - (normal and -SD and -CH <sub>2</sub> D species) - Ethyl mercaptan - 45	$C_7H_7F$ - $(CHD_2C_6H_4F)$ - $\alpha_{d_2}$ -Orthofluorotoluene - 50
$C_6H_6S$ - Thiophenol, thiophenol-SD - 7	$C_7H_7BrO$ - m-Br-anisole - 6
$C_6H_6Se$ - Selenophenol-SeD - 7	$C_7H_7NO_3$ - m-NO <sub>2</sub> -anisole - 6
$C_6H_7N$ - $(C_6H_5NH_2)$ - Aniline - 7, 9	$C_7H_7F$ - $(CH_2DC_6H_4F)$ - $\alpha_{d_1}$ -Parafluorotoluene - 50
$C_6H_7N$ - Methylene cyclobutyl cyanide - 12	$C_7H_7F$ - $(CHD_2C_6H_4F)$ - $\alpha_{d_2}$ -Parafluorotoluene - 50
$C_6H_7P$ - Phenylphosphine - 7	$C_7H_8$ - Toluene - 23

- C<sub>7</sub>H<sub>8</sub> - (CH<sub>2</sub>DC<sub>6</sub>H<sub>5</sub>) - d<sub>1</sub>-Toluene - 50
- C<sub>7</sub>H<sub>8</sub>O - Bicyclo(2.2.1)hept-2-ene-5-one - 35
- C<sub>7</sub>H<sub>8</sub>O - Bicyclo[2,2,1]hept-2-ene-7-one - 38
- C<sub>7</sub>H<sub>8</sub>O - Tricyclo(2.2.1.0<sup>2,6</sup>)heptanone - 35
- C<sub>7</sub>H<sub>8</sub>S - Endo- and exo-2,3-epithio-5-norbornene - 36
- C<sub>7</sub>H<sub>10</sub> - Δ<sup>6</sup>Bicyclo(3.2.0.)heptene - 21
- C<sub>7</sub>H<sub>10</sub>O - Bicyclo(2.2.1)heptan-2-one - 35
- C<sub>7</sub>H<sub>10</sub>O - Bicyclo[2,2,1]heptane-7-one - 38
- C<sub>7</sub>H<sub>10</sub>O - Exo-3-oxatricyclo(3.2.1.0<sup>2,4</sup>)-octane - 35
- C<sub>7</sub>H<sub>10</sub>O - Norbornanone - 12
- C<sub>8</sub>H<sub>6</sub> - Phenyl acetylene - 3
- C<sub>8</sub>H<sub>7</sub>Br - Br-styrenes - 7
- C<sub>8</sub>H<sub>7</sub>Cl - m-Cl-styrene - 6
- C<sub>8</sub>H<sub>7</sub>Br - m-Br-styrene - 6
- C<sub>8</sub>H<sub>7</sub>NO<sub>2</sub> - m-NO<sub>2</sub>-styrene - 6
- C<sub>8</sub>H<sub>7</sub>F - p-Fluorostyrene - 41
- C<sub>8</sub>H<sub>9</sub>Cl - m-Cl-ethylbenzene - 6
- C<sub>8</sub>H<sub>9</sub>Br - m-Br-ethylbenzene - 6
- C<sub>8</sub>H<sub>9</sub>I - m-I-ethylbenzene - 6
- C<sub>8</sub>H<sub>10</sub>S - 9-Thia-bicyclo[3.3.1]-nona-2,6-diene - 9
- C<sub>8</sub>H<sub>11</sub>N - N-ethylaniline - 6
- C<sub>8</sub>H<sub>12</sub>O - Bicyclo(2.2.2)octanone - 35
- C<sub>9</sub>H<sub>10</sub>O - Propiophenone - 6
- C<sub>9</sub>H<sub>10</sub>O - p-Ethylbenzaldehyde - 6
- C<sub>9</sub>H<sub>10</sub>O - Bicyclo[3.2.2]-nona-6,8-diene-3-one - 9
- C<sub>9</sub>H<sub>14</sub>O - Exo,exo-5,6-dimethyl-norcamphor - 11
- C<sub>9</sub>H<sub>14</sub>O - Endo-exo-5,6-dimethyl-norcamphor - 11
- C<sub>9</sub>H<sub>14</sub>O - Endo-endo-5,6-dimethyl-norcamphor - 11
- C<sub>9</sub>H<sub>14</sub>O - Exo-endo-5,6-dimethyl-norcamphor - 11
- C<sub>10</sub>H<sub>12</sub>O - p-i-Propylbenzaldehyde - 6
- C<sub>10</sub>H<sub>12</sub>O - 8-Ketotricyclo[5.2.1.0<sup>2,6</sup>]-4-decene - 11
- C<sub>10</sub>H<sub>14</sub>O - 8-Ketotricyclo[5.2.1.0<sup>2,6</sup>]decane - 11
- C<sub>10</sub>H<sub>14</sub>O - Tricyclo(3.3.1.1<sup>3,7</sup>)decanone - 35
- C<sub>10</sub>H<sub>15</sub>N - p-i-Propyl-N-methylaniline - 6
- C<sub>10</sub>H<sub>17</sub>Cl - l-Bornyl chloride - 11
- C<sub>11</sub>H<sub>20</sub>O - 1-Bornyl-methyl ether - 11
- C<sub>12</sub>H<sub>18</sub>O<sub>2</sub> - cis-2-Acetoxy-pin-3-ene - 11
- C<sub>12</sub>H<sub>20</sub>O<sub>2</sub> - 1-Bornylacetate - 11
- CaF - Calcium Fluoride - 4
- ClCs - (CsCl) - Cesium chloride - 2
- ClHO<sub>4</sub> - (HOClO<sub>3</sub>) - Perchloric acid - 14
- ClNO - Nitrosyl chloride - 27
- ClO - Chlorine monoxide - 14
- CrF<sub>2</sub>O<sub>2</sub> - Chromyl fluoride - 52
- Cl<sub>3</sub>OP - (POCl<sub>3</sub>) - Phosphorus trichloride - 15
- CsI - Cesium iodide - 2
- CsF - Cesium fluoride - 2
- CuF - Copper monofluoride - 2
- FGa - (GaF) - Gallium monofluoride - 2

FNO - (NOF) - Nitrosyl fluoride - 13, 17, 27    PbS - Lead sulphide - 2  
F<sub>2</sub>HNSO - (HN=S(O)F<sub>2</sub>) - Imidosulfuryl fluoride - 20    SnS - Tin sulphide - 2  
F<sub>2</sub>S - (SF<sub>2</sub>) - Sulfur difluoride - 14  
F<sub>3</sub>H<sub>3</sub>Si<sub>2</sub> - (SiF<sub>3</sub>SiH<sub>3</sub>) - Trifluoro silane - 39  
F<sub>3</sub>PO - Phosphoryl fluoride - 27  
F<sub>4</sub>OS - (F<sub>4</sub>SO) - Sulfur oxytetrafluoride - 52  
F<sub>4</sub>S - (SF<sub>4</sub>) - Sulfur tetrafluoride - 14  
F<sub>5</sub>I - (IF<sub>5</sub>) - Iodine pentafluoride - 15  
GeS - Germanium sulphide - 2  
HNC - Hydrogen isocyanide - 54  
HO - (OH) - Hydroxyl radical - 5, 31  
HOCl - Hypochloric acid - 13  
HNO<sub>2</sub> - Nitrous acid - 34  
H<sub>3</sub>N - Ammonia - 50  
LiNa - Sodium lithium - 4, 29  
NO<sub>2</sub> - Nitrogen dioxide - 4, 5  
N<sub>2</sub>D<sub>4</sub> - Hydrazine - 12  
N<sub>2</sub>O<sub>3</sub> - Dinitrogen trioxide - 20  
OS - (SO) - Sulfur monoxide - 24  
OS<sub>2</sub> - (S<sub>2</sub>O) - Disulfur monoxide - 24  
OS<sub>2</sub> - (S<sub>2</sub>O) - Disulfur oxide - 2  
OSe - (SeO) - Selenium oxide - 5  
O<sub>2</sub> - Oxygen - 14  
O<sub>2</sub>S<sub>2</sub> - (OSSO) - SO-dimer - 24  
O<sub>3</sub>+CH<sub>2</sub>=CH<sub>2</sub> - Ozonides - 43