

HARVARD UNIVERSITY  
Department of Chemistry  
12 Oxford Street  
Cambridge, Massachusetts 02138

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Dear Contributor:

This is the twelfth microwave spectroscopy information letter and is being sent to those who contributed:

1. UNIVERSITY OF BOLOGNA  
Istituto Chimico "G. Ciamician"  
P.O. Favero

$CF_2O$	Carbonyl fluoride		in press.
$H_2Se(D_2Se)$	Deuterium selenide.		Dipole moment. in press
$H_2Se(D_2Se)$	Deuterium selenide		Millimeter wave spectrum in progress.
$COCl_2$	Carbonyl chloride		Millimeter wave spectra in progress.
$HOClO$	Hypochlorous acid		Millimeter wave spectra in progress.

2. BOWDOEN COLLEGE  
Chemistry Department  
S. S. Butcher

$C_2H_4F_2 (CH_2FCH_2F)$	1,2-difluoroethane	S. S. Butcher	Ground state and anti-tilts assigned. Isotopic work in progress.
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3. UNIVERSITY OF MICHIGAN  
School of Chemistry  
Dr. A. Peter Cox

$CH_3NO_2$	Nitromethane	R. E. Mackaman	Isotopic work in progress.
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$\text{CH}_3\text{NO}_2$	Methyl nitrate	S. Waring	Oxygen-18 in progress.
$\text{C}_4\text{H}_9\text{NOSi} [(\text{CH}_3)_3\text{SiNCO}]$	Trimethyl silicon isocyanate		Assigned.
$\text{C}_4\text{H}_9\text{NSi} [(\text{CH}_3)_3\text{SiNCS}]$	Trimethyl silicon isothiocyanate		Assigned.
$\text{C}_5\text{H}_5\text{NiNO} [(\text{C}_5\text{H}_5)_2\text{NiNO}]$	Cyclopentadienyl nitrosyl nickel	A.H. Wittain	In manuscript. Vibrational analysis in progress.
$\text{C}_5\text{H}_5\text{PtNO} [(\text{C}_5\text{H}_5)_2\text{PtNO}]$	Cyclopentadienyl nitrosyl platinum	C. Roberts	Notes in preparation.
$\text{C}_5\text{H}_5\text{Ti} )$ $\text{C}_5\text{D}_5\text{Ti} )$	Cyclopentadienyl thallium	C. Roberts	Manuscript in preparation
$\text{HNO}_2$	Nitrous acid	A.H. Wittain	In manuscript. Centrifugal distortion nearly complete.
$\text{N}_2\text{O}_3$	Dinitrogen trioxide	A.H. Wittain (see R.L. Kuezhorst)	Accepted for publication
		D.J. Finnigan	Quadrupole coupling near completion.

4. UNIVERSITY OF CALIFORNIA, SANTA BARBARA  
Department of Chemistry  
David O. Harris

$\text{C}_3\text{H}_6\text{Se}$	trimethylene selenide	M. Petit	Spectrum assigned for 6 vibrational states, barrier determined
$\text{C}_3\text{F}_6\text{O}_2$	dioxolane	P. Baron	Spectrum assigned for 9 pseudorotation states
CN	CN radical	P. Meakin	Reanalysis of spectrum complete
$\text{C}_4\text{H}_6\text{O}$	2-methylene oxetane	J. Gibson	Spectrum assigned for 6 vibrational states, potential determined.

5. UNIVERSITY OF COPENHAGEN  
 Department of Chemistry Physics  
 Lorge Bak/Lise Nygaard

$C_3H_3NS$	thiazole		4- $^{13}C$ - and 5- $^{13}C$ - species assigned, r <sub>s</sub> - structure.
$C_3H_3N_2$	pyrazole		4-D-species assigned.
$C_4H_5N$	pyrrole		in press.
$C_4H_6$	cyclobutene		in press.
$C_6H_5NO_2$	nitrobenzene	J.H. H <sub>yg</sub>	assignment incl. Q- lines and satellites
$C_6H_6O$	phenol		in press.
$C_7H_5N$	benzonitrile	J. Casado G.O. Sørensen	reinvestigation incl. Q-lines and centrifugal distortion.

6. UNIVERSIDAD NACIONAL DE LA PLATA  
 Department of Physics  
 L.M. Boggia/O.H. Sorarrain

$C_{10}H_8$	Azulene	L.M. Boggia C. Gomez	Assignments made. Structure in progress.
$C_4H_9NS$	Thiomorpholine	R. Veronesi M.C. Villani	Research in progress
$C_3H_4O_2$	β-propiolactone	L. Boggia O. Sorarrain	Spectrum assigned. Vib- rational states measured.
$C_4H_8S_2[S(CH_2)_2]_2$	p-dithiane	C. Villani C. Gomez	Research in progress.
$C_4H_9NO[NH(CH_2)_2 O(CH_2)_2]$	morpholine	O. Sorarrain C. Gomez	Research in progress

7. UNIVERSITY OF FREIBURG  
Physikalisches Institut  
H.D. Rudolph

$C_2H_3NS (CH_3SCN)$	Methyl-thiocyanate	H. Schleser	5 isotopic species spectra assigned, $r_e$ -structure, quadrupole efg. constants.
$C_2H_2NS (CD_3SCN)$	$d_3$ -methyl-thiocyanate	H. Heimburger	Spectrum assigned; work continued after 1 year intermission.
$C_2H_6S [(CH_3)_2S]$	Diethyl-sulfide } Dimethyl-silane }	A. Trinkaus	Barrier potential from excited torsional states, in press.
$C_2H_6Si [(CH_3)_2SiH_2]$			
$C_4H_6O [(CH_3)_2COO]$	Dimethyl-ketene	H. Dreizler I. Rosenbaum H.D. Rudolph	Partial structure, barrier; 0-15 in preparation.
$C_7H_9 (CD_3C_6H_5)$	$d_3$ -toluene	A. Kreiner	Work commenced.
$C_8H_{10} [(C_2H_5)_2C_6H_4]$	Ortho-xylene	H.D. Rudolph	Ground state spectrum evaluated; excited torsional states.

8. GEORGIA INSTITUTE OF TECHNOLOGY  
School of Physics  
T.L. Weatherly/Q. Williams

$SCl_2$	Sulfur Dichloride	W.A. Little	Manuscript in preparation
$CH_2Br_2$	Dibromomethane	F. Tsai	Spectrum observed and tentatively assigned.

9. UNIVERSITY OF GLASGOW  
Department of Chemistry  
J.K. Tyler

$C_2H_2NO (HOCH_2CN)$	Glycolonitrile	D.G. Lister	Main and OD species assigned. Quadrupole coupling.
$C_2H_3N (NH_2CH_2CN)$	Aminoacetonitrile	J.N. Macdonald	Measurements extended to H- deuterio species

$\text{CH}_2\text{N}_2$ ( $\text{NH}_2\text{CN}$ )	Cyanamide	J.N. Macdonald	Perturbed Q-branch lines measured. Stark effect analysed for $\mu$ .
$\text{C}_5\text{H}_4\text{O}_3$	Pyron-4-thione	E. Manley	$^{34}\text{S}$ and ring deuterio species in progress.
$\text{C}_6\text{H}_6\text{FN}$ ( $\text{FC}_6\text{H}_5\text{NH}_2$ )	p-fluoroaniline	R.L. MacNeil A. Hastie	Measurements extended to deuterated species.
$\text{C}_6\text{H}_7\text{N}$ ( $\text{C}_6\text{H}_5\text{NH}_2$ )	Aniline	D.G. Lister J.K. Tyler	r <sub>g</sub> structure nearly complete.

10. HARVARD UNIVERSITY  
Department of Chemistry  
E.B. Wilson

$\text{C}_2\text{H}_4\text{F}_3\text{N}$ ( $\text{CF}_3\text{CH}_2\text{NH}_2$ )	Trifluoroethylemine	I. Warren	spectrum assigned
$\text{C}_2\text{H}_4\text{O}$ ( $\text{CH}_3\text{CHO}$ )	acetaldehyde	C.R. Parent	barrier
$\text{C}_2\text{H}_3\text{ClO}$ ( $\text{CH}_2\text{ClCHO}$ )	chloroacetaldehyde	R. Ford	cis form assigned
$\text{C}_3\text{H}_8\text{O}$ [ $(\text{CH}_3)_2\text{HCOH}$ ]	isopropanol	P. Larson	partial assignment
$\text{CH}_4\text{N}_2$ ( $\text{DNHCH}_3$ )	trans methyl diimide	W. Steinmetz	spectrum assigned
$\text{CN}$ ( $\text{ICN}$ )	cyanogen iodide	J. Cohen	energy transfer
$\text{C}_2\text{H}_5\text{NO}_3$ ( $\text{HOCH}_2\text{CH}_2\text{NO}_2$ )	2-nitroethanol	M. Fuller	in progress.

11. HEWLETT-PACKARD COMPANY  
Microwave Spectroscopy Laboratory  
L.H. Scharpen/H.W. Harrington

$\text{C}_n\text{H}_{2n+1}\text{X}$	n-Alkyl halides n=3; X=Cl, Br, I n=4; X=Cl, Br, I n=5; X=Br, I n=6; X=F, I	near symmetric-top spectra; (B+C) values for two rotamers each.
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$C_7H_7X[(C_6H_5)CH_2X]$	Benzyl derivatives	near symmetric-top spectra; (B+C) values for two rotamers each.
$C_5H_8O_3W$	$[C_5H_5W(CO)_2CH_2]$	symmetric-top like spectra assigned
$C_8H_6O_3W$	$[C_5H_5W(CO)_2R]$	symmetric-top like spectra assigned
$C_6F_3MnO_5$	$[CF_3Mn(CO)_3]$	symmetric-top like spectra assigned
$C_6H_{11}F$	Cyclohexyl fluoride	axial-equatorial energy difference determined.
$C_3H_5F$	3-Fluoropropene $[CH_2=CH(CH_2F)]$	Measurement of vibrational and conformational energy differences in progress.

12. UNIVERSITY OF KANSAS  
Department of Chemistry  
M.P. Harmony

$C_4H_6$	Bicyclobutane	In press
$C_3H_5N(C_2H_5CN)$	Ethyl cyanide	In press
$C_3H_7N(C_3H_5NH_2)$	Cyclopropylamine	In press
$C_5H_7Cl$	1-chloro bicyclo[1.1.1] pentane	In progress
$C_4H_8N(C_4H_6NH_2)$	Cyclobutylamine	In progress
$C_2H_5NO$	N-methyl formamide	In progress

12a. UNIVERSITY DE LILLE  
 Departement de Physique  
 R. Wertheimer

$\text{CH}_2^{16}\text{O}_2$	Formic Acid	Samson	Centrifugal distortion analysis; deuterated species; search for rotamers.
$\text{Cl}_2^{35}\text{O}_2$	Thionyl chloride	Journal	Ground state partially assigned for $\text{SO}^{35}\text{Cl}_2$ , $\text{SO}^{35}\text{Cl}^{37}\text{Cl}$ .
$\text{C}_4\text{H}_8\text{O}_4$	Tetraoxane	Colmont	
$\text{C}_2\text{H}_3\text{N}$ ( $\text{CH}_3\text{CN}$ )	Acetonitrile	Bauer	Vibrationally excited states.
$\text{C}_3\text{H}_6\text{O}_3$	Trioxane	Colmont	Excited vibrational states.
$\text{CH}_3\text{Br}$	Methyl bromide	Lemaire	Excited vibrational states.

13. LOUISIANA STATE UNIVERSITY IN NEW ORLEANS 70122  
 Department of Physics  
 E.L. Reeson, Jr.

$\text{CCL}_2\text{F}_2$	Dichlorodifluoromethane	Shu-Ming Hu	Analyzing nuclear quadrupole splitting
$\text{C}_3\text{H}_7\text{N}$	Propylene imine	R. Schmidt	Studying hyperfine splitting and internal rotation of <u>cis</u> isomer.

14. UNIVERSITE DE LOUVAIN  
 Institut de physique Nucleaire Parc d'Arenberg  
 M. de Hemptinne

$\text{C}_2\text{H}_6\text{O}$ ( $\text{CH}_3\text{CH}_2\text{OH}$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$\text{C}_2\text{H}_6\text{O}$ ( $\text{CH}_3^{13}\text{CH}_2\text{OH}$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$\text{C}_2\text{H}_6\text{O}$ ( $\text{CH}_3\text{CH}_2^{18}\text{OH}$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$\text{C}_2\text{H}_5\text{DO}$ ( $\text{CH}_3\text{CHDOH}$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$\text{C}_2\text{H}_5\text{O}$ ( $\text{CH}_3\text{CH}_2\text{O}$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned

$C_2H_5DO$ ( $CH_2DCH_2OH$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$C_2H_4D_2O$ ( $CH_2CD_2OH$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$C_2H_2D_3O$ ( $CD_2CH_2OH$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$C_2HD_4O$ ( $CD_2CD_2OH$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$C_2D_6O$ ( $CD_2CD_2OH$ )	Ethyl alcohol	J.P. Culot	Spectrum assigned
$C_2H_3Br$ ( $CH_2CHBr$ )	Vinyl bromide	D. de Kerckhove	Spectrum assigned
$C_2H_2DBr$ ( $CH_2CDBr$ )	Vinyl bromide	J. Marroor	Spectrum assigned
$C_2H_2D_2Br$ ( $CHDCHBr$ )	Vinyl bromide	D. de Kerckhove	Spectrum assigned
$C_2H_2D_3Br$ ( $CDECHBr$ )	Vinyl bromide	D. de Kerckhove	Spectrum assigned
$SO_2$ ( $^{32}S^{16}O_2$ )	Sulfur Dioxide	G. Steinbecklier	2d order distribution for fundamental and excited states.
$SO_2$ ( $^{33}S^{16}O^{17}O$ )	Sulfur Dioxide	R. Van Riet and G. Steinbecklier	Spectrum assigned
$SO_2$ ( $^{33}S^{16}O^{17}O$ )	Sulfur Dioxide	G. Steinbecklier	Spectrum assigned
$SO_2$ ( $^{33}S^{16}O^{18}O$ )	Sulfur Dioxide	G. Steinbecklier	Spectrum assigned
$SO_2$ ( $^{33}S^{17}O^{17}O$ )	Sulfur Dioxide	G. Steinbecklier	Spectrum assigned
$SO_2$ ( $^{33}S^{18}O^{18}O$ )	Sulfur Dioxide	G. Steinbecklier	Spectrum assigned
$SO_2$ ( $^{33}S^{17}O^{18}O$ )	Sulfur Dioxide	G. Steinbecklier	Spectrum assigned



15. MCDONNELL DOUGLAS CORPORATION  
McDonnell Research Laboratories  
J. Wollrab

$C_2H_4N_2Cl$	Methylchlorodiazirine	with L.H. Scherpen	complete
$C_2H_7N$	Dimethylamine (torsional states)	with V.W. Laurie	in writing
$C_2H_4SO$	Ethylene Episulfoxide (excited states)	with W.P. White	several states assigned.
$C_3H_9N$	Trimethylamine	with V.W. Laurie	$r_s$ structure

16. UNIVERSITY OF MANCHESTER  
Physics Department  
Dr. J.G. Baker

$C_2F_3N$ ( $CF_3CN$ )	Trifluoroacetonitrile	M.J. Whittle	paper on excited bending states in preparation.
$C_2H_3N$ ( $CH_3CN$ )	Acetonitrile	M.J. Whittle	"
$F_3OP$	Phosphorus oxyfluoride	M.J. Whittle	"
$BrF_5$	Bromine pentafluoride	M.J. Whittle	Work commenced
$C_3H_6F_2$	2,2-difluoropropane	B. Weiss	In progress
$C_3H_7F$	2-fluoropropane	B. Weiss	In progress
$Br_3P$	Phosphorus tribromide	J.G. Baker	Computer analysis of spectra.
$C_{12}H_{10}O$	Diphenyl ether	J.G. Baker	Computer analysis of spectra.

17. UNIVERSITY OF MARYLAND  
 Institute for Molecular Physics  
 L.C. Krisher

$C_4H_2O_3$	Maleic anhydride	L.C. Krisher J. Sheridan (Wales)	Assigned
$C_2H_2FO$	Fluoroacetylene	E.I. Saegbarth L.C. Krisher	One form, manuscript in preparation
$C_2H_4N_2O$	Methyl-furazan	E.I. Saegbarth	Assigned, intermediate barrier
$C_3H_6O$	2-methylfuran	W.G. Norris L.C. Krisher	In press
$C_5H_6S$	2-methylthiophene	S. Wolf	In progress
$C_5H_4O_3$	Citraconic anhydride	S. Wolf L.C. Krisher	In progress
$C_2H_3NO$ and $C_2D_3H_3NO$	Acetamide	E.I. Saegbarth L.C. Krisher	Temporarily abandoned

18. UNIVERSITY OF MICHIGAN  
 Department of Chemistry  
 R. Kuczkowski

$H_2O_3$	Dinitrogen Trioxide	R. Kuczkowski	Vib. satellites
$BF_2NH_2$ ( $H_2$ , $BPF_2H$ )	Difluorophosphine-Borane	J. Pasinski	3 isotopes done
$C_3H_{12}$ $BPF_3(CH_3)_3$	Trimethylphosphine-Borane	P. Bryan	3 isotopes done
$C_3H_{12}$ $BPF_3[(CH_3)_3NH_3]$	Trimethylamine-borontri-fluoride	P. Bryan	4 isotopes done

19. MICHIGAN STATE UNIVERSITY  
 Department of Chemistry  
 R. H. Schwendeman

$C_3H_5O_2$ ( $CH_2CH_2COO$ ) 	Cyclopropylcarboxylic acid fluoride	J.N. Volltrauer	Manuscript in preparation
$C_3H_4O$ ( $CH_2CH_2CHO$ ) 	Cyclopropylcarboxaldehyde	H.N. Volltrauer	Manuscript in preparation
$C_3H_6$ ( $CH_2CH_2CH_2$ ) 	Vinylcyclopropane	E.G. Coddling	Manuscript in preparation
$C_3H_4O_2$ ( $CH_2COCHO$ ) 	Glycidaldehyde	R.H. Schwendeman	Nearly complete
$C_4H_8O$ ( $CH_2CH_2CH_2CO$ ) 	Methylcyclopropyl ketone	P. Lee	Assigned
$C_2H_5NO$ ( $HCN(CH_3)_2$ ) 	Dimethylformamide	H.B. Thompson	Assigned

20. NATIONAL BUREAU OF STANDARDS  
 Molecular Spectroscopy  
 W.H. Kirchhoff

$BrO$	Bromine monoxide	D.R. Johnson F.X. Powell	$2^2P_{3/2}$ state in press $2^2P_{1/2}$ state under investigation.
$CN$ ( $HCN$ )	Hydrogen Cyanide	A. Maki	$C^{13}, N^{15}$ excited vibrational states
$CF_2$	Carbon difluoride	F.X. Powell W.H. Kirchhoff	Centrifugal Distortion under investigation
$CO_2$	Carbonyl Sulfide	A. Maki	$C^{13}, O^{18}$ excited vibrational states
$C_2HBF_2$ ( $HC \equiv C-BF_2$ )	Ethynyldifluoroborane	W. Lafferty	$B^{10}, B^{11}$ assigned manuscript in preparation

$C_4H_6S$ ( $\underline{S-CH_2-CHCHCH_2}$ )	2,5 dihydrothiophene	J. Greenhouse	planar molecule, puckering states assigned.
$C_4H_6S$ ( $\underline{SCHCHCH_2CH_2}$ )	2,3 dihydrothiophene	J. Greenhouse	non-rigid rotor, assigned.
$C_4H_{10}S_2$ ( $\underline{S-CH_2-CH_2-CH_2-CH_2-S}$ )	Dithiacyclopentane	W. Lafferty J. Durig	ring atom substitution, puckering vibration, manuscript in preparation.
$ClF_5$	Chlorine pentafluoride	W. Kirchhoff	dipole moment measured.
$Cl_3FO$	Trichloroamine Oxide	D.R. Lide W.H. Kirchhoff	Dipole Moment in press
$F_2S$	Sulfur difluoride	F.X. Powell D.R. Johnson	in press, centrifugal distortion in progress.

21. NATIONAL RESEARCH COUNCIL OF CANADA  
Division of Pure Physics  
C. C. Costain

$H_2S_2$ (HSSH)	Hydrogen Disulfide	G. Winnewisser	mm spectrum assigned
$D_2S_2$ (DSSD)	Deuterium Disulfide	G. Winnewisser	mm spectrum assigned

22. UNIVERSITY OF NEW BRUNSWICK

Chemistry and Physics  
W.V.F. Brooks/R.M. Lees

$CH_4O$ ( $CH_3OH$ )	Methyl alcohol	R.M. Lees	Spectrum assigned of deuterated species
$C_3H_6S$ ( $CH_2=CHCH_2SH$ )	Allyl Mercaptan	S.C. Dass A. Bhaumik	Paper accepted for -S-H and -S-D species
$C_4H_8O$ ( $\underline{CH_2-CH_2-CH-CH_2OH}$ )	Cyclopropyl Carbinol	W.V.F. Brooks K.V.L.N. Sastry	Manuscript in preparation for -O-H and -O-D species

$C_3H_3N_3$ ( $C_3N_3H_3$ )	1,2,4-triazine	A. Bhaumik S.C. Dass	Ground State Assigned
$C_2ON_2$ ( $CO(CN)_2$ )	Carbonyl cyanide	R.M. Lees	Quadrupole splitting analysis.

23. STATE UNIVERSITY OF NEW YORK AT BUFFALO  
Department of Physics  
T.M. Jarochman

$C_3H_7Br$ ( $CH_3CH_2CH_2Br$ )	Normal propyl bromide		manuscript in preparation
$C_3H_7I$ ( $CH_3CH_2CH_2I$ )	Normal propyl iodide		spectrum assigned

24. UNIVERSITY OF OSLO  
Department of Chemistry  
K.M. Barstok/H. Kallendal

$C_3BrN$ ( $BrCCCN$ )	Bromocynoacetylene	T. Bjorvatten	$r_s$ structure complete
$C_3ClN$ ( $ClCCCN$ )	Chlorocynoacetylene	T. Bjorvatten	$r_s$ structure complete
$C_3IN$ ( $ICCCN$ )	Iodocynoacetylene	T. Bjorvatten	Normal, $^{13}C$ , and $^{15}N$ species done
$C_4HCl$ ( $HCCCCl$ )	Monochlorodiacetylene	A. Bjørseth	Spectrum assigned
$C_2BrCl$ ( $BrCCCl$ )	Chlorobromodiacetylene	A. Bjørseth	Spectrum assigned
$C_2ClI$ ( $ICCCl$ )	Chloriododiacetylene	A. Bjørseth	Spectrum assigned
$C_2H_4O_2$ ( $H_2C(OH)CHO$ )	Glycolaldehyde	H. Kallendal	Spectrum assigned

$C_2H_4O_2(H_2C(OD)CHO)$  d-Glycolaldehyde H. Møllendal Spectrum assigned

25. THE PENNSYLVANIA STATE UNIVERSITY  
Chemistry Department  
L. P. Gold

$C_2H_2N_2Se$  1,3,4-selenadiazole D. Levine  $^{80}Se, ^{78}Se$  species in  
W. Krugh press (J.Mol.Spectry.)  
( $\underline{CH=N-N=CH-Se}$ ) Other species in progress

$C_2H_6OS$  methyl vinyl sulfoxide W. Krugh In progress  
( $CH_2SOCH=CH_2$ )

$CH_5As$  methyl arsine D. Levine In progress  
( $CH_3AsH_2$ )

26. II. PHYSIKALISCHES INSTITUT  
Freie Universität Berlin  
R. Honerjäger

In	Indium-monofluoride	F. Lovas T. Torring	In press
AgF	Silver-monofluoride	F. Lovas T. Torring	Rotational spectrum, dipole moment
OPb	Lead-monoxide	J. Hoefft	Dipole moments and rota- tional spectra completed
PbS	Lead-monosulfide	F. Lovas	
OSn	Tin-monoxide	E. Tiemann	
SSn	Tin-monosulfide	R. Tischer	
GeO	Germanium-monoxide	T. Torring	
GeS	Silicium-monosulfide	T. Torring	
SSi	Silicium-monosulfide	T. Torring	
PbTe	Lead-monotelluride	J. Hoefft E. Tiemann B. Stender	In press
InI	Indium-iodide	B. Stender	Quadrupole coupling

27. PRINCETON UNIVERSITY  
Department of Chemistry  
V.W. Laurie

$C_3H_6$	Methylene cyclopropane	W. Stigliani	3 isotopic species assigned
$C_2H_7N$ ( $CH_3CH_2NH_2$ )	Ethylamine	Y.S. Li	Q-branch assigned
$INO$	nitrous oxide	L. Scharpen	polarizability measured
$CH_2C \equiv CH$	methyl acetylene	J. Kuenter	
$(CH_3)_2GeH_2$	Dibethylgermane	E.C. Thomas	In press
$C_5H_{10}Ge$	germacyclopentane	E.C. Thomas	Completed

28. RICE UNIVERSITY  
Department of Chemistry  
R. Curl

$C_2H_7NO$ ( $CH_3CH_2CH_2OH$ )	Ethanolamine	R. Penn	Several isotopic species assigned
$C_3CH_2O$ ( $CH_2CHCOCl$ )	Acryloyl Chloride	David Hemphill	Trans isomer assigned
$ClO_2$	Chlorine dioxide	Ray Mariella	$V_2 = 1$ vibrational state analysis

29. UNIVERSITY OF SOUTHERN CALIFORNIA  
Department of Chemistry  
R. A. Beaudet

$C_2H_6B_2$	2,3 dicarbahexaborane	R.L. Poynter R.A. Beaudet	Manuscript
$C_3H_3N$ ( $CH_2 = CHN$ )	Vinyl isocyanide	W.C. Cumming	Draft
$C_3H_5Br$ ( $CH_2CH = CHBr$ )	<u>cis</u> bromopropene	R.A. Beaudet Zaida Luthey	Draft

$C_3H_6F_2$ $(CH_3)_2CF_2$	2,2 difluoropropane	R.A. Beaudet R.I. Poynter	Vibrational states
$C_3H_6F_2Si$ $(CH_2CH_2CF_2SiH_2)$	Difluoro sila cyclobutane	R.G. Ford	Draft
$C_3H_6B_2$ $(CH_3)_2B_2H_4$	2-methyl-1,6-dicarbaborane-2-borane	L. Wang	Structure
$C_4H_6O$ $(CH_2=CHCH_2CH_2O)$	tetraene monoxide	W.C. Cummings	Assigned
$C_4H_6O$ $((CH_3)_2CCH_2O)$	1,1-dimethylethylene oxide	W.C. Cummings	Assigned
$C_5H_6F_2$ $(CF_2=CHC(CH_3)=CH_2)$	3-methyl-1,1 difluoro-butadiene	T.S. Huang	Submitted
$C_5H_6F_2$ $[CF_2=C(CH_3)CH=CH_2]$	2-methyl-1,1 difluoro-butadiene	W.C. Cummings	Draft
$C_5H_8$ $(CH=C(CH_3)CH_2CH_2)$	1-methylcyclobutene	T.S. Huang	Draft
$C_5H_6$ $(CH_3CH=CHC\equiv CH)$	<u>cis</u> 3-pentene-1-yne	R.G. Ford	Draft
$B_2C_2H_5Cl$	2 chloro-1,6 dicarbaborane (6)	G. McKown	Completing isotopic species
$C_3H_4F_2O$ $(CH_2CF_2CH_2O)$	B,B difluorooxetane	G. McKown	Completing intensities
$CD_3BF_2$	methyl boron difluoride	S. Cheung	Manuscript submitted
$C_3H_7P$ $[(CH_3)CH_2CH_2PH]$	propylene phosphine	M.T. Bowers R.A. Beaudet	Manuscript submitted
$C_3H_7F$ $[CH_3CH_2P(CH_3)]$	P-methyl phosphirane	M.T. Bowers R.A. Beaudet	Partially assigned



29a. UNIVERSITY OF TEXAS  
Department of Chemistry  
J.E. Boggs

$\text{CH}_3^{\text{D}}$ ( $\text{CH}_2^{\text{H}}\text{PH}_2$ )	Methyl phosphine	R. Young	Spectra of deuterated species assigned.
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30. UNIVERSITY OF TOKYO  
Department of Chemistry  
Y. Morino

$\text{CH}_2^{\text{D}}\text{F}_2$ $\text{CH}_2^{\text{D}}\text{F}_2$	Methylene fluoride	K. Sakakibara	Centrifugal distortion; work completed.
$\text{CH}_3^{\text{D}}$ ( $\text{CH}_2^{\text{H}}\text{NH}_2$ )	Methyl amine-d	K. Tamagaki	Trans and gauche assigned
$\text{C}_2\text{H}_4\text{OS}$ [( $\text{CH}_2$ ) <sub>2</sub> SO]	Ethylene episulfoxide	S. Saito	In press (Bull. Chem. Soc. Japan)
$\text{C}_3\text{H}_5\text{Cl}$	Allyl chloride	E. Hirota	Cis and skew assigned; work almost completed.
$\text{C}_3\text{H}_7\text{O}$ [( $\text{CH}_2$ ) <sub>2</sub> COH]	Isopropyl alcohol	S. Kondo	Trans and gauche assigned; manuscript in preparation.
$\text{C}_4\text{H}_8$	Cis-butene-2	S. Kondo	Manuscript in preparation
$\text{C}_5\text{H}_8$ ( $\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$ )	1,4-Pentadiene	E. Hirota	One rotamer assigned.
$\text{CH}_3\text{F}$ ( $\text{HCCl}$ )		T. Beppu	Manuscript in preparation.
$\text{ClO}$	Chlorine monoxide	T. Amano	In press (J. Mol. Spectr.)
$\text{FNO}_2$	Nitryl fluoride	T. Tanaka	Manuscript in preparation
$\text{F}_2^{\text{D}}$ ( $\text{PF}_3$ )	Phosphorous trifluoride	E. Hirota	Vib-rot interactions; work completed

$\text{H}_3\text{N} (\text{ND}_3)$	Ammonia- $\text{d}_3$	T. Urisu	Direct l-doublet in $1/4$ ; manuscript in preparation.
HS	Nitrogen sulfide	T. Amano	In Press (J.Mol.Spectro)
$\text{O}_2$	Oxygen	T. Amano	Manuscript in preparation
$\text{O}_2\text{S} (\text{SO}_2)$	Sulfur dioxide	S. Saito	In press (J.Mol.Spectro)
$\text{O}_2\text{Se} (\text{SeO}_2)$	Selenium dioxide	H. Takeo	Manuscript in preparation
$\text{O}_3$	Ozone	T. Tanaka	Manuscript in preparation

31. TOKYO INSTITUTE OF TECHNOLOGY  
 Laboratory of Chemical Spectroscopy  
 K. Kozima

$\text{C}_4\text{H}_4 (\text{CH}_2\text{CH=CH})$	Vinylacetylene	C. Hirose	Vibrational satellites, two states assigned.
$\text{C}_4\text{H}_3\text{D} (\text{CH}_2\text{CH=CD})$	Vinylacetylene	C. Hirose	G.S. and vibrational satellites assigned. Fermi and Coriolis res.
$\text{C}_4\text{H}_6\text{O} (\text{CH}_3\text{CH=CHCHO})$	trans-crotonaldehyde	M. Suzuki	In press
$\text{C}_4\text{H}_6\text{O} (\text{CH}_2\text{C}(\text{CH}_3)\text{CHO})$	Methacrolein	M. Suzuki	Manuscript in preparation
$\text{C}_5\text{H}_8 (\text{CH}_2\text{CH=CHCH=CH}_2)$	1,3-pentadiene	M. Suzuki	Manuscript in preparation
$\text{C}_4\text{H}_5\text{N} (\text{CH}_2\text{C}(\text{CH}_3)\text{CN})$	Methacrylonitrile	M. Suzuki	Manuscript in preparation
$\text{C}_5\text{H}_6 (\text{CH}_2\text{C}(\text{CH}_3)\text{CCH})$	2-methyl-1-butene-3-yne	M. Suzuki	Manuscript in preparation
$\text{C}_5\text{H}_7 (\text{CH}_3\text{CH=CHCN})$	trans crotonitrile	M. Suzuki	Manuscript in preparation

$C_6H_{10}$	$(\underline{CH_2CH_2CH_2CH_2CHCH})$	Cyclohexene	T. Ogata	In press (Bull. Chem. Society. Japan)
$C_5H_6O$	$(\underline{CH_2CHOCCH_2(CH_2)})$	cyclopentenone	T. Ogata	Work in progress

32. UNIVERSITY COLLEGE LONDON  
Department of Chemistry  
H. J. Allen

HO $F$		Nitrosyl fluoride	K.C. Buchton A.C. Legon	Paper accepted
WF $Cl_5$		Tungsten chloride pentafluoride	A.C. Legon	Paper submitted
HO $Cl$		Hypochlorous acid	D.C. Lindsey D. Lister	Spectrum assigned. Preliminary structure obtained
$C_5H_6O$		2-cyclo-pentene-one	D. Chadwick A.C. Legon	Spectrum assigned
CH $_2Br_2$		Methylene bromide	D. Chadwick	Spectrum assigned
$C_{10}H_{15}CN$		Admantyl cyanide	D. Chadwick A.C. Legon	Spectrum assigned

33. UNIVERSITY COLLEGE OF NORTH WALES, BANGOR  
Department of Chemistry  
J. Sheridan

$C_3H_5N$		propargyl amine	K. Bolton	3 isotopic forms
$C_2H_3N$		vinyl isocyanide	K. Bolton	$\mu_0, \mu_1$ ; vibrational satellites; infrared vibrational assignment, paper ready.
$C_3H_4O_2$		acrylic acid	K. Bolton	cis/trans energy difference; shape of cis/trans P.E. function; paper in preparation.

$C_6H_4O_2$	o-quinone	K. Bolton	orientating experiments on volatility/stability problem in heated cell.
$C_3H_4N_2$	imidazole	J.H. Griffiths	5 isotopic forms dipole direction N-coupling tensors.
$C_3H_7F$	isopropyl fluoride	J.H. Griffiths	refined treatment of V. vibrational assignment
$C_2HBr$	bromo acetylene	H. Jones	12 isotopic forms, r <sub>g</sub> structure, l-doublets, dipole
$C_2H_3N_3$	1,2,3-triazole	H. Jones O.L. Stiefvater	double resonance-double search assignment; paper nearly ready; results communicated to Dr. L. Nygaard, Copenhagen, where detailed structure study is planned.
$C_4H_3N$	propargyl cyanide	H. Jones	Assignment
$C_5H_9OF$	Trimethylacetyl fluoride	H. Jones O.L. Stiefvater	Assignment
$C_3H_6O$	cyclopropanol	J. Marks	work continuing
$C_2H_3NO$	Acetonitrile-N-oxide	J. Marks	Orientating experiments on volatility/stability problem.
$C_3H_3NS$	Isothiazole	A. Wardley	Several isotopic forms; N-coupling; $\mu_a, \mu_b$ .
$C_2H_3O_2X$	substituted methyl formates (X=F, CN, CCH, cis-CH:CH <sub>2</sub> , CH <sub>3</sub> )	G. Williams	barriers; vibrational assignments; dipoles; papers in preparation.
$C_2H_2N_2O$	2,4-oxadiazole	V. Williams	N-coupling constants
$C_2H_3HSe$	isoselenazole	V. Williams	$\mu_a, \mu_b$ , N-coupling
$C_5H_8O$	2,3-dihydropyran	V. Williams	$\mu$ , vibrational satellites
$C_4H_8O$	isobutyraldehyde	O.L. Stiefvater	gauche form assigned; $\mu$ , 8 excited states, search for second rotamer.

$C_4H_7OF$	isobutyryl fluoride	T.D. Summers O.L. Stiefvater	Abundant rotamer and several excited states assigned
$C_3H_6O_2$	Propionic acid	O.L. Stiefvater	cis-form completed, search for second rotamer resumed.
$C_2DF, CHD_2F$	Methyl fluoride	M. Takami	1 mm spectra, refined constants
$C_2HCl$	Chloroacetylene	M. Takami H. Jones	1 mm spectra, refined constants, $\lambda$ -doublets
$CH_2O$	Formaldehyde	M. Takami	R-branch lines to sub-mm range†
$C_2H_3N$	Methyl isocyanide	M. Takami	1 mm spectra refined constants; refined vibrational satellite analysis†
$C_4H_8O$	Ethyl Vinyl ether	N.L. Owen	Barrier calculated for one rotamer.
$C_3H_6O_3$	Dimethyl carbonate	N.L. Owen	Work continuing
$C_7H_7OF$	p-fluoroanisole	N.L. Owen	Many lines measured, work continuing

† work on these being continued by Dr. Takami at Institute of Physical and Chemical Research, Yamato-Machi, Japan

34. UNIVERSITY OF WISCONSIN *54306*  
Department of Chemistry  
R.C. Woods

$C_4H_{10}O$	t-butylalcohol	Valenzuela	In progress
$C_2H_4O_2 (CH_2OHCHO)$	Glycolaldehyde	Simons	In progress

35. UNIVERSITY OF WISCONSIN AT MADISON  
Department of Chemistry  
C.D. Cornwell

$B_2BrH_5 (B_2H_5Br)$	Brossodiborane	A.C. Ferguson	Manuscript in preparation
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$\text{BrF}_5$	Bromine pentafluoride	J. Grow	In progress
$\text{F}_5\text{I}$ ( $\text{IF}_5$ )	Iodine pentafluoride	J. Grow	In progress

Later Additions:

36. SWISS FEDERAL INSTITUTE OF TECHNOLOGY  
Laboratory of Physical Chemistry  
Hs.H. Günthard

$\text{C}_2\text{H}_3\text{NO}_2$ ( $\text{CH}_2 = \text{CHNO}_2$ )	Nitroethylene	P. Nosberger	Excited states
$\text{C}_3\text{H}_5\text{I}$ ( $\text{CH}_2 = \text{CICH}_3$ )	2-Iodopropene	A. Bauder	Ground state complete, first excited state studied
$\text{C}_3\text{H}_7\text{N}$ ( $\text{CH}_3\text{CH} = \text{NCH}_3$ )	N-Methylethylidenimine	J. Meier	Spectra measured
$\text{C}_3\text{H}_4\text{N}_2\text{O}_2$ ( $\text{CH}_2\text{CNCH}_2\text{NO}_2$ )	Nitroacetonitrile	M. Ribaud	Spectrum measured

37. UNIVERSITÄT ULM  
Lehrstuhl für Physikalische Chemie  
W. Zeil

$\text{CH}_3\text{SiH}_2\text{Cl}$	Methyl chloro silane	R. Ronchi W. Zeil	Spectrum assigned
$(\text{CH}_3)_2\text{SiHCl}$	Dimethyl chloro silane	Heinz Jetter W. Zeil	Spectrum assigned
$\text{C}_2\text{H}_5\text{SiH}_2\text{Cl}$	Ethyl chloro silane	Volker Typke W. Zeil	Work in progress

38. INSTITUT FÜR PHYS.-CHEMIE  
UNIVERSITÄT FRANKFURT  
W. Winkle

$(\text{CH}_3)_3\text{-C-Hal}$	Tert. Butyl-Halides	W. Winkle	Spectra assigned.
$(\text{HF})_n$	Fluoric Acid	U. Reinert	Building up the spectrograph
$\text{SiH}^{37}\text{Cl}_2$	Trichlorsilan	G. Loos	Preparation of $^{37}\text{Cl}$ .

39. LAVAL UNIVERSITY, QUEBEC, QUEBEC, CANADA  
Department of Chemistry  
P. Buckley

$C_7H_5NO$   
( $NOCH_2CH_2OH$ )      2-cyanoethanol      P. Buckley      Partially assigned;  
trans and gauche isomers  
observed.

40. MOWASH UNIVERSITY\*  
Department of Chemistry  
R.D. Brown, F.R. Burden, J.E. Kent

$C_6H_6$       3,4-dimethylene cyclobutene      B. Hart      Isotopic spectrum  
assigned

$C_6H_6$       3,4-dimethylene cyclobutene      G. Blackman      Zeeman spectrum  
observed

$C_6H_6$       Fulvene      J. Kent      Isotopic work under-  
way

$C_8H_8$       Styrene and fluoro styrenes      M. Fuller      Spectra observed

$C_6H_5N_2O$       Benzoxadiazole      G. Mohay      Spectrum assigned

$C_2H_3NO$       Acetonitrile-n-oxide      I. Gillard      Spectrum assigned

$C_R F_4$       Chromium tetrafluoride      P. Burton      Spectrum assigned

$C_4H_4Te$       Tellurophen      P. Godfrey      Spectrum assigned

\* This was a late contribution, therefore, the formula's are not  
listed in the formular index.

## FORMULA INDEX

- AgF Silver-monofluoride - 26
- BF<sub>2</sub>H<sub>4</sub>P (H<sub>2</sub>BPF<sub>2</sub>H) Difluorophosphine-Borane - 18
- B<sub>2</sub>BRH<sub>5</sub> (B<sub>2</sub>H<sub>5</sub>Br) Bromodiborane - 35
- BrF<sub>5</sub> Bromine pentafluoride - 16, 35
- BrO Bromine monoxide - 20
- Br<sub>3</sub>P Phosphorus tribromide - 16
- COCl<sub>2</sub>O (COCl<sub>2</sub>) Carbonyl chloride - 1
- CF<sub>2</sub> Carbon difluoride - 20
- CF<sub>2</sub>O Carbonyl fluoride - 1
- CCl<sub>2</sub>F<sub>2</sub> Dichlorodifluoromethane - 13
- CHN (HCN) Hydrogen Cyanide - 20
- CH<sub>2</sub>Br<sub>2</sub> Dibromomethane (methylene bromide) - 8, 32
- CH<sub>2</sub>F<sub>2</sub> (CD<sub>2</sub>F<sub>2</sub>) Methylene fluoride - 30
- CH<sub>2</sub>N<sub>2</sub> (NH<sub>2</sub>CN) Cyanamide - 9
- CH<sub>2</sub>O Formaldehyde - 33
- CH<sub>3</sub>F (CH<sub>2</sub>DF, CHD<sub>2</sub>F) Methyl fluoride - 33
- CH<sub>3</sub>NO<sub>2</sub> Nitromethane - 3
- CH<sub>3</sub>NO<sub>3</sub> Methyl nitrate - 3
- CH<sub>4</sub>N<sub>2</sub> (DNNCH<sub>3</sub>) trans methyldiimide - 10
- CH<sub>4</sub>O (CH<sub>2</sub>OH) methyl alcohol - 22
- CH<sub>5</sub>As (CH<sub>3</sub>AsH<sub>2</sub>) Methyl arsine - 25
- CH<sub>5</sub>ClSi (CH<sub>3</sub>SiH<sub>2</sub>Cl) Methyl chlorosilane - 37
- CH<sub>5</sub>N (CH<sub>2</sub>DNH<sub>2</sub>) Methyl amine-d - 30
- CH<sub>5</sub>P (CH<sub>2</sub>PH<sub>2</sub>) Methyl phosphine - 29a
- C<sub>2</sub>BrCl (BrCCCl) Chlorobromoacetylene - 24
- C<sub>2</sub>ClI (ICCCl) Chloriodoacetylene - 24
- C<sub>2</sub>F<sub>3</sub>N (CF<sub>3</sub>CN) Trifluoroacetonitrile - 16
- C<sub>2</sub>HBF<sub>2</sub> (HC≡C-BF<sub>2</sub>) Ethynyl difluoro borane - 20
- C<sub>2</sub>HBr Bromo acetylene - 33
- C<sub>2</sub>HCl Chloroacetylene - 33
- C<sub>2</sub>H<sub>2</sub>N<sub>2</sub>O 2,4-oxadiazole - 33
- C<sub>2</sub>H<sub>2</sub>N<sub>2</sub>Se (CH=N-N=CH-Se) 1,3,4-selenadiazole - 25
- C<sub>2</sub>H<sub>3</sub>Br (CH<sub>2</sub>CHBr) Vinyl Bromide - 14
- C<sub>2</sub>H<sub>3</sub>ClO (CH<sub>2</sub>ClCHO) Chloroacetaldehyde - 10
- \*(insert at bottom)
- C<sub>2</sub>H<sub>3</sub>N (CH<sub>3</sub>CN) Acetonitrile - 16
- C<sub>2</sub>H<sub>3</sub>N Methyl isocyanide - 33
- C<sub>2</sub>H<sub>3</sub>NO Acetonitrile-N-oxide - 33  
40
- C<sub>2</sub>H<sub>3</sub>NO (HOCH<sub>2</sub>CN) Glycollonitrile - 9
- C<sub>2</sub>H<sub>3</sub>NO<sub>2</sub> (CH<sub>2</sub>=CHNO<sub>2</sub>) Nitroethylene - 36
- C<sub>2</sub>H<sub>3</sub>NS (CH<sub>3</sub>SCN) Methyl-thiocyanate - 7
- C<sub>2</sub>H<sub>3</sub>N<sub>2</sub>Cl Methylchlorodiazirine - 15
- C<sub>2</sub>H<sub>3</sub>N<sub>3</sub> 1,2,3-triazole - 33
- C<sub>2</sub>H<sub>4</sub>F<sub>2</sub> (CH<sub>2</sub>FCH<sub>2</sub>F) 1,2-difluoroethane - 2
- \* C<sub>2</sub>H<sub>3</sub>NO<sub>2</sub> (CH<sub>3</sub>COO) Methyl nitroacetate - 33



- $C_2H_4F_3N$  ( $CF_3CH_2NH_2$ ) Trifluoroethylamine - 10
- $C_2H_4N_2$  ( $NH_2CH_2CN$ ) Aminoacetonitrile - 9
- $C_2H_4O$  ( $CH_3CHO$ ) Acetaldehyde - 10
- $C_2H_4OS$  [ $(CH_2)_2SO$ ] Ethylene episulfoxide - 30,15
- $C_2H_4O_2$  ( $CH_2OHCHO$ ) Glycolaldehyde - 34, 24
- $C_2H_5B_4Cl$  ( $B_4C_2H_5Cl$ ) 2 chloro-1,6-dicarbahexaborane(6) - 29
- $C_2H_5NO$  N-methyl formamide - 12
- $C_2H_5NO$  Acetamide - 17
- $C_2H_6B_4$  2,3-dicarbahexaborane - 29
- $C_2H_6O$  ( $CH_3CH_2OH$ ) Ethyl alcohol - 14
- $C_2H_6S$  [ $(CH_3)_2S$ ] Dimethyl sulfide - 7
- $C_2H_7ClSi$  ( $C_2H_5SiH_2Cl$ ) Ethyl chlorosilane - 37
- $C_2H_7ClSi$  [ $(CH_3)_2SiHCl$ ] Dimethyl chlorosilane - 37
- $C_2H_7N$  ( $CH_3CH_2NH_2$ ) Ethylamine - 27
- $C_2H_7N$  Dimethylamine (torsional states) - 15
- $C_2H_7NO$  ( $NH_2CH_2CH_2OH$ ) Ethanolamine - 28
- $C_2H_8Si$  [ $(CH_3)_2SiH_2$ ] Dimethyl silane - 7
- $C_2H_8Ge$  [ $(CH_3)_2GeH_2$ ] Dimethylgermane - 27
- $C_3BrN$  ( $BrCCCN$ ) Bromocyanoacetylene - 24
- $C_3ClN$  ( $ClCCCN$ ) Chlorocyanoacetylene - 24
- $C_3IN$  ( $ICCCN$ ) Iodocyanoacetylene - 24
- $C_3N_2O$  [ $CO(CN)_2$ ] Carbonyl cyanide - 22
- $C_3H_3ClO$  ( $CH_2CHCOCl$ ) Acryloyl chloride - 28
- $C_3H_3N$  ( $CH_2=C=CHN$ ) Vinyl isocyanide - 22, 23
- $C_3H_3NO_2$  Methyl Cyanofornate - 33  
( $CH_3OCOCN$ )
- $C_3H_3NS$  Isothiazole - 33
- $C_3H_3N_2$  Thiazole - 5
- $C_3H_3N_2S$  Isoselenazole - 33
- $C_3H_3N_3$  ( $C_3N_3H_3$ ) 1,2,4-triazine - 22
- $C_3H_4$  ( $CH_3C\equiv CH$ ) Methyl acetylene - 27
- $C_3H_4F_2O$  ( $CH_2CF_2CH_2O$ )  $\beta, \beta$  difluorooxetane - 29
- $C_3H_4N_2$  Imidazole - 33
- $C_3H_4N_2$  Pyrazole - 5
- $C_3H_4N_2O$  Methyl-furazan - 17
- $C_3H_4N_2O_2$  ( $CH_3ONCH_2NO_2$ ) Nitroacetonitrile - 36
- $C_3H_4O_2$  Acrylic acid - 33
- $C_3H_4O_2$  ( $CH_2OCHCHO$ ) Glycidaldehyde - 19
- $C_3H_4O_2$   $\beta$ -propiolactone - 6
- $C_3H_5Br$  ( $CH_3CH=CHBr$ ) cis bromopropene - 29
- $C_3H_5Cl$  Allyl chloride - 30
- $C_3H_5F$  ( $CH_2=CHCH_2F$ ) 3-Fluoropropene - 11
- $C_3H_5FO$  Fluoroacetone - 17
- $C_3H_5I$  ( $CH_2=CICH_3$ ) 2-Iclopropene - 36
- $C_3H_5N$  ( $C_2H_5CN$ ) Ethyl cyanide - 12
- $C_3H_5N$  Propargyl amine - 33
- $C_3H_5F_2$  [ $(CH_3)_2CF_2$ ] 2,2-difluoropropane - 29
- $C_3H_5F_2$  1,1-difluoropropane - 29

- $C_3H_6F_2Si$  ( $\underline{CH_2CH_2CH_2SiF_2}$ ) Difluoro sila-cyclobutane - 29
- $C_3H_6O$  Cyclopropanol - 33
- $C_3H_6OS$  ( $CH_3SOCH=CH_2$ ) Methyl vinyl sulfoxide - 25
- $C_3H_6O_2$  Dioxolane - 4
- $C_3H_6O_2$  ( $CH_3OCOCH_3$ ) Methyl Acetate - 33
- $C_3H_6O_2$  Propionic Acid - 33
- $C_3H_6O_3$  Dimethyl carbonate - 33
- $C_3H_6S$  ( $CH_2=CHCH_2SH$ ) Allyl Mercaptan - 22
- $C_3H_6Se$  Trimethylene selenide - 4
- $C_3H_7Br$  ( $CH_3CH_2CH_2Br$  Normal Propyl Bromide - 11, 23
- $C_3H_7Cl$  N,propyl chloride - 11
- $C_3H_7F$  2-fluoropropane - 16,33
- $C_3H_7I$  ( $CH_3CH_2CH_2I$ ) Normal Propyl Iodide - 23, 11
- $C_3H_7N$  ( $C_3H_5NH_2$ ) Cyclopropylamine - 12
- $C_3H_7N$  ( $CH_3CH=NCH_3$ ) N-methylethyliacnimine - 36
- $C_3H_7N$  Propylene imine - 13
- $C_3H_7NO$  [ $HCON(CH_3)_2$ ] Dimethylformamide - 19
- $C_3H_8B_3$  ( $CH_3 \cdot B_3C_2H_5$ ) 2-methyl-1,5-dicarbapentaborane - 29
- $C_3H_8O$  [ $(CH_3)_2CHOH$ ] Isopropyl alcohol - 10,30
- $C_3H_{12}BP$  [ $(CH_3)_3PBH_3$ ] TRimethyl phosphine-Borane - 18
- $C_3H_3N$  Trimethylamine - 15
- $C_3H_{12}BP$  [ $(CH_3)_3PBH_3$ ] TRimethyl phosphine-Borane - 18
- $C_4HCl$  ( $HCCCCl$ ) Monochlorodiacylene - 24
- $C_4H_2O_3$  Maleic anhydride - 17
- $C_4H_3N$  Propargyl cyanide - 33
- $C_4H_4$  ( $CH_2CHCCH$ ) Vinylacetylene - 31
- $C_4H_4O_2$  ( $HCCCO_2CH_3$ ) Methyl Propynate - 33
- $C_4H_5FO$  ( $\underline{CH_2CH_2CHCOF}$ ) Cyclopropyl-carboxylic acid fluoride - 19
- $C_4H_5N$  ( $CH_3CHCHCN$ ) trans crotononitrile - 31
- $C_4H_5N$  ( $CH_2C(CH_3)CN$ ) Methacrylonitrile - 31
- $C_4H_5N$  Pyrrole - 5
- $C_4H_6$  Bicyclobutane - 12
- $C_4H_6$  Cyclobutene - 5
- $C_4H_6$  Methylene Cyclopropane - 27
- $C_4H_6O$  ( $CH_2=CHCHCH_2O$ ) Butadiene monoxide - 29
- $C_4H_6O$  ( $CH_3CHCHCHO$ ) trans crotonaldehyde - 31
- $C_4H_6O$  ( $\underline{CH_2CH_2CHCHO}$ ) Cyclopropyl-carboxaldehyde - 19
- $C_4H_6O$  [ $(CH_2)_2CCO$ ] Dimethyl-ketene-7
- $C_4H_6O$  [ $CH_2C(CH_3)CHO$ ] Methacrolein-31
- $C_4H_6O$  3-Methylene oxetane - 4
- $C_4H_6O_2$  ( $CH_2CHCO_2CH_3$ ) Methyl cis propenate - 33
- $C_4H_6S$  ( $\underline{SCHCHCH_2CH_2}$ ) 2,3 dihydrothiophene - 20
- $C_4H_6S$  ( $\underline{SCH_2CHCHCH_2}$ ) 2,5 dihydrothiophene - 20
- $C_4H_7FO$  Isobutyryl fluoride - 33
- $C_4H_8$  cis 2-butene - 30
- $C_4H_8N$  ( $C_4H_8NH_2$ ) Cyclobutylamine - 17
- $C_4H_8O$  ( $\underline{CH_2CH_2CHCH_2OH}$ ) Cyclopropyl Carbinol - 22

- $C_4H_8O$   $[(CH_3)_2CCH_2O]$  1,1-dimethylethylene oxide - 29
- $C_4H_8O$  Ethyl vinyl ether - 33
- $C_4H_8O$  Isobutyraldehyde - 33
- $C_4H_8S_2$   $[S(CH_2)_2]_2$  p-dithiane - 6
- $C_4H_9Br$  N-butyl bromide - 11, 38
- $C_4H_9Cl$  N-butyl chloride - 11, 38
- $C_4H_9I$  N-butyl iodide - 11, 38
- $C_4H_9NO$   $[NH(CH_2)_2O(CH_2)_2]$  morpholine - 6
- $C_4H_9NOSi$   $[(CH_3)_3SiNCO]$  Trimethyl silicon isocyanate - 3
- $C_4H_9NS$  Thiomorpholine - 6
- $C_4H_9NSSi$   $[(CH_3)_3SiNCS]$  Trimethyl silicon isothiocyanate - 3
- $C_4H_{10}Ge$  Germacyclopentane - 27
- $C_4H_{10}O$  T, butyl alcohol - 34
- $C_4H_{10}OSi$   $(SiH_2CH_2CH_2CH_2CH_2)$  Silacyclopentane - 20
- $C_5H_4OS$  Pyran-4-thione - 9
- $C_5H_4O_3$  Citraconic anhydride - 17
- $C_5H_5NNiO$   $(C_5H_5NiNO)$  Cyclopentadienyl nitrosyl nickel - 3
- $C_5H_5NOPt$   $(C_5H_5PtNO)$  Cyclopentadienyl nitrosyl platinum - 3
- $C_5H_5Tl$  Cyclopentadienyl thallium - 3
- $C_5H_6$   $(CH_2C(CH_3)CCH)$  2-methyl-1-butene-3-yne - 32
- $C_5H_6$   $(CH_3C\equiv CHC\equiv CH)$  cis 3-pentene-1-yne - 29
- $C_5H_6F_2$   $[CF_2=CHC(CH_3)=CH_2]$  1-methyl-1,1-difluorobutadiene - 29
- $C_5H_6O$  2-methylfuran - 17
- $C_5H_6O$   $[(CH_2)_4C=O]$  2-pyrone - 17
- $C_5H_6O$  2-cyclo-pentene-one - 32
- $C_5H_6S$  2-methylthiophene - 17
- $C_5H_7Cl$  1-chloro bicyclo(1.1.1)pentane - 12
- $C_5H_8$   $[\overline{CH=C(CH_3)CH_2CH_2}]$  1-methylcyclobutene - 29
- $C_5H_8$   $(CH_3CHCHCHCH_2)$  1,3-pentadiene - 31
- $C_5H_8$   $(CH_2=CHCH_2CH=CH_2)$  1,4-Pentadiene - 30
- $C_5H_8$   $(\overline{CH_2CH_2CHCHCH_2})$  Vinylcyclopropane - 19
- $C_5H_8O$   $(\overline{CH_2CH_2CHCOCH_3})$  Methylcyclopropyl ketone - 19
- $C_5H_8O$  2,3-dihydropyran - 33
- $C_5H_9FO$  Trimethylacetyl fluoride - 33
- $C_5H_{11}Br$  N-pentyl bromide - 11
- $C_5H_{11}I$  N-pentyl iodide - 11
- $C_5F_3MnO_5$   $(CF_3Mn(CO)_5)$  - 11
- $C_6H_4O_2$  O-quinone - 33
- $C_6H_5NO_2$  Nitrobenzene - 5
- $C_6H_6FN$   $(FC_6H_4NH_2)$  p-fluoroaniline - 9
- $C_6H_6O$  Phenol - 5
- $C_6H_7N$   $(C_6H_5NH_2)$  Aniline - 9
- $C_6H_{10}$   $(\overline{CH_2CH_2CH_2CH_2CHCH})$  Cyclohexene - 31
- $C_6H_{11}F$  Cyclohexyl fluoride - 11
- $C_6H_{13}F$  N-hexyl fluoride - 11
- $C_6H_{13}I$  N-hexyl iodide - 11
- $C_7H_5N$  Benzonitrile - 5
- $C_7H_7Br$   $(C_6H_5CH_2Br)$  Benzyl Bromide - 1

$C_7H_7I$ ( $C_6H_5CH_2I$ ) Benzyl Iodide - 10	GeO Germanium-monoxide - 26
$C_7H_7FO$ p-fluoroanisole - 33	GeS Germanium-monosulfide - 26
$C_7H_8$ $d_3$ -toluene - 7	$(HF)_n$ Fluoric Acid - 38
$C_8H_8O_3W$ ( $C_5H_5W(CO)_3H$ ) - 11	$HNO_2$ Nitrous acid - 3
$C_8H_7N$ ( $C_6H_5CH_2CN$ ) Benzyl Cyanide - 10	$H_2S_2$ (HSSH) Hydrogen Disulfide - 23
$C_8H_{10}$ [ $(CH_3)_2C_6H_4$ ] Ortho-xylene - 7	$H_2Se$ Deuterium selenide - 1
$C_9H_8O_3W$ ( $C_5H_5W(CO)_3CH$ ) <sub>3</sub> - 11	$H_3N$ Ammonia- $d_3$ - 30
$C_{10}H_8$ Azulene - 6	IIIn INdium-iodide - 26
$C_{11}H_{15}N$ ( $C_{10}H_{15}CN$ ) Adamantyl cyanide - 32	NS Nitrogen sulfide - 30
$C_{12}H_{10}O$ Diphenyl ether - 16	$N_2O$ (NNO) nitrous oxide - 27
CIN (ICN) Cyanogen iodide - 10	$N_2O_3$ Dinitrogen Trioxide - 3,18
CN CN Radical - 4	OPb Lead-monoxide - 26
COS Carbonyl Sulfide - 20	OSn Tin-monoxide - 26
$ClF_5$ Chlorine pentafluoride - 20	$O_2$ OXYgen - 30
$ClF_5W$ Tungsten chloride pentafluoride - 32	$O_2S$ ( $SO_2$ ) Sulfur dioxide - 14,30
$ClHO$ (HClO) Hypochlorous acid - 1,32	$O_2Se$ ( $SeO_2$ ) Selenium dioxide - 30
$ClNS$ (NSCl) - 30	$O_3$ Ozone - 30
$ClO$ Chlorine monoxide - 30	PbS Lead-monosulfide - 26
$ClO_2$ Chlorine dioxide - 28	PbTe Lead-monotelluride - 26
$Cl_2S$ ( $SCl_2$ ) Sulfur Dichloride - 8	SSi Silicium-monosulfide - 26
$Cl_3HSi$ ( $SiH^37Cl_3$ ) Trichlorosilane - 38	SSn Tin-monosulfide - 26
FIIn INdium-monofluoride - 26	
$FNO$ (NOF) Nitrosyl fluoride - 32	
$FNO_2$ Nitryl fluoride - 30	
$F_2S$ Sulfur difluoride - 20	
$F_3NO$ Trifluoramine Oxide - 20	
$F_3P$ ( $PF_3$ ) Phosphorous trifluoride - 30	
$F_2OP$ Phosphorus oxyfluoride - 16	
$F_5I$ ( $IF_5$ ) Iodine pentafluoride - 35	

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$C_5H_6Se$	2-Methylthiophene	nearly complete
$C_4H_4Se$	selenophene	$r_s$ structure
$C_4H_8Se$	tetrahydro selenophene	$r_s$ structure $5^s$ isotopes

Unfortunately these formulas were not included in the index.