

MICROWAVE SPECTROSCOPY INFORMATION LETTER

VOL. LXII

April 15, 2019

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MICROWAVE SPECTROSCOPY NEWSLETTER LXI

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In Memoriam

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(Written by Angela Hight Walker)

Walt Lafferty

(Written by Wallace "Pete" Pringle and Bill Kirchhoff)

Li-Hong Xu

(Written by Yunjie Xu, Jens-Uwe Grabow, and Shui-Ming Hu)

Interesting and Informative Websites Maintained by Our Colleagues and Funding Acknowledgement

1. The J. P. L. *Submillimeter, Millimeter, and Microwave Spectral Line Catalog* is accessible via anonymous ftp at spec.jpl.nasa.gov or via our home page at <http://spec.jpl.nasa.gov>
Jet Propulsion Laboratory, **Lab 9**.
2. A database "Programs for ROTational SPEctroscopy (PROSPE)" is available at:
<http://info.ifpan.edu.pl/~kisiel/prospe.htm>
A new database on "History of Rotational Spectroscopy" is being constructed at:
<http://info.ifpan.edu.pl/~kisiel/rothist/rothist.html>
A subpage on this Newsletter is at:
<http://info.ifpan.edu.pl/~kisiel/rothist/newsletter.html>
This database depends critically on contributions, which are solicited and accepted at (preferably): prospe@ifpan.edu.pl, **Lab 22**
3. Recommended Rest Frequency Table. F. J. Lovas, *J. Phys. Chem. Ref. Data*, 1-181 (2004). See:
<http://physics.nist.gov/PhysRefData/micro/html/contents.html>
For diatomics, triatomics, and hydrocarbons, see:
<http://physics.nist.gov/PhysRefData/MolSpec/index.html>
A graphic, interactive fitting program, jb95, is available at
<http://physics.nist.gov/Divisions/Div844/facilities/uvs/jb95userguide.htm>
An application and description of the program is found in D. F. Plusquellic et al., *J. Chem. Phys.*, 115 (2001) 3057.
National Institute of Standards and Technology, **Lab 32**.
4. A bibliography of high resolution studies of weakly bound complexes is maintained on the Web at
<http://www.Wesleyan.edu/chem/faculty/novick/vdw.html>
Wesleyan University, **Lab 36**.
5. The Cologne Database for Molecular Spectroscopy is available online at
<http://www.astro.uni-koeln.de/cdms/>
I. Physikalisches Institut, Köln, **Lab 34**.
6. The Hannover FTMW spectrometer control & analysis software is available at
<http://www.pci.uni-hannover.de/~lgpca/spectroscopy/ftmw>
Institut für Physikalische Chemie, Hannover, **Lab 13**.

Garry Grubbs II would like to thank the Missouri University of Science and Technology Chemistry Department and College of Arts, Sciences, and Business for covering the cost of all printing and shipping of this volume of the Microwave Spectroscopy Information Letter.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₆ N ₂ O	Glycinamide ^{b,d}		ApJ 861:70 (7pp), 2018
C ₂ H ₃ NO	Methyl isocyanate ^{a,b,d}		mmw-sub wave spectrum
C ₂ H ₄ O ₂	Vinyl Alcohol		mmw-sub wave spectrum
C ₂ H ₃ NO	Propynal		mmw-sub wave spectrum
C ₃ H ₃ NO	Propiolamide ^d		mmw-sub wave spectrum
C ₃ H ₃ NO ₂	Cyanoacetic acid		spectrum assigned
C ₃ H ₅ NO	Ethylisocyanide ^a		A&A 616, A173 (2018)
C ₃ H ₆ O ₂	Metoxyacetaldehyde ^a		A&A 619, A67 (2018)
C ₃ H ₆ O ₂	Lactaldehyde		ms. in preparation
C ₃ H ₃ NO ₃	2,5-oxazolidinedione		JPCL,10,1325(2019)
C ₃ H ₆ N ₂ O ₃	Hydantoic Acid		JPCL,10,1325(2019)
C ₃ H ₇ N ₃ O ₂	Glycociamine		LA-MBFT spectrum
C ₃ H ₉ NO ₂	N-methyl alanine		PCCP 20, 29159 (2018)
C ₄ H ₂ O ₄	Squaric acid		ms. in preparation
C ₄ H ₄ O ₆	Malic acid		ms. In preparation
C ₄ H ₆ O ₆	Tartaric Acid		ms. in preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₇ N ₃ O	Creatinine ^{e,f}		ms. in preparation
C ₄ H ₇ N ₃ O ₃	Cytosine-water		ms. in preparation
C ₄ H ₉ NO ₂	Aminoisobutyric Acid		Chem. E.J., 25, 2288 (2019)
C ₄ H ₉ NO ₂	3-Aminobutyric Acid		PCCP 20,15574 (2018)
C ₄ H ₉ NO ₂ S	Homocysteine		ms. in preparation
C ₄ H ₉ NO ₃	Homoserine		LA-CPFT/LA-MBFT spectrum
C ₄ H ₁₀ O ₄	Erythritol		LA-CPFT spectrum
C ₅ H ₁₀ N ₂ O ₂	Glutamine		ms. in preparation
C ₅ H ₁₀ O ₅	Arabinose		ms. in preparation
C ₅ H ₁₀ O ₅	Lixose		ms. in preparation
C ₅ H ₁₀ N ₂ O ₃	Alanine-Glycine		LA-CPFT spectrum
C ₅ H ₁₁ NO	Norvaline		LA-CPFT spectrum
C ₅ H ₁₁ NO ₂	Isovaline		ms. in preparation
C ₅ H ₁₁ NO ₂ S	Methionine		ms. in preparation
C ₅ H ₁₂ O ₅	Ribitol ^c		Chem. Eur.J., 25,2288 (2019)
C ₅ H ₁₂ O ₅	Arabitol		LA-CPFT spectrum
C ₅ H ₁₂ O ₅	Xylitol		LA-CPFT spectrum
C ₆ H ₁₀ NO ₂	Pipecolic Acid		PCCP 21, 4155 (2019)
C ₆ H ₁₂ O ₆	Mannose		ms. in preparation
C ₆ H ₁₄ O ₆	Dulcitol		ChemPhysChem 2018,19,3334
C ₆ H ₁₂ O ₆	Sorbitol		ChemPhysChem 2018,19,3334
C ₆ H ₁₂ O ₆	Manitol		LA-CPFT spectrum

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₁₂ O ₆	Inositol		LA-CPFT spectrum
C ₆ H ₁₂ N ₂ O ₃	Alanyl alanine		LA-CPFT spectrum
C ₇ H ₅ NO ₃ S	Saccharin		JPCA (2019)
C ₇ H ₁₂ N ₂ O ₃	Prolylglycine		LA-CPFT spectrum
C ₇ H ₁₂ N ₂ O ₃	Glycylproline		Comm. Chemistry (2019)
C ₈ H ₈ O ₃	Mandelic acid		LA-CPFT spectrum
C ₈ H ₈ O ₄	Dopac		LA-CPFT spectrum
C ₈ H ₉ NO ₃	Pyridoxal (Vit. B6)		ms. In preparation
C ₈ H ₁₁ NO ₃	Pyridoxine (Vit. B6)		ms. In preparation
C ₈ H ₁₁ NO ₃	Noradrenaline		LA-MB-FTMW spectrum
C ₉ H ₁₂ N ₂ O ₂	Dulcine		LA-CPFT spectrum
C ₉ H ₁₂ N ₂ O ₅	Deoxyuridine		LA-MB-FTMW spectrum
C ₉ H ₁₃ NO ₃	Adrenaline		ms. In preparation
C ₁₂ H ₁₆ N ₂	N,N-Dimethyltryptamine		LA-CPFT spectrum
C ₁₂ H ₂₂ O ₁₁	Sucrose		LA-CPFT spectrum
C ₁₂ H ₂₂ O ₁₁	Lactose		LA-CPFT spectrum
C ₁₉ H ₂₈ O ₂	Testosterone		LA-CPFT spectrum

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH ₅ FO	Methylfluoride-H ₂ O	Sharon Priya Gnanasekar Manuel Goubet, Robert Georges	Assigned transitions for hydrogen bond structure. Carbon bonded structure?
CH ₃ ArF	Argon-methylfluoride	Sharon Priya Gnanasekar Manuel Goubet, Robert Georges	Assigned transitions for a T-shaped structure. Several unassigned lines C--Ar and F--Ar structures?
H ₄ S ₂	H ₂ S dimer	Arijit Das, Chris Medcarft Frank J. Lovas, Pankaj Mandal, Nick R. Walker	Angew. Chem. Int. Ed. Engl. K 57, 15199 (2018)
C ₃ H ₃ NO ₂	Acetonitrile-CO ₂ dimer	Sharon Priya Gnanasekar	K = 0 lines of a T-shaped Structure similar HCN-CO ₂ assigned. Stacked structure is assigned.
H ₄ NeO ₂	Ne-(H ₂ O) ₂	Arijit Das	20Ne lines of one progression assigned and fitted. Search for ²² Ne lines and other tunneling states in progress.
C ₉ H ₈ O	phneylpropargylether	Kabir R Kumbhar	Spectrum assigned.
C ₃ H ₅ O ₂	propargyl alcohol-H ₂ O	Sharon Priya Gnanasekar	Spectrum assigned

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
$C_6H_8N_2$ ($C_5H_4N-CH_2NH_2$)	2-Picolylamine	R. Bird	Experiments Completed Assignments In Progress
$C_6H_8N_2$ ($C_5H_4N-CH_2NH_2$)	3-Picolylamine	R. Bird	Experiments Completed Assignments In Progress
$C_6H_8N_2$ ($C_5H_4N-CH_2NH_2$)	4-Picolylamine	R. Bird	Experiments Completed Assignments In Progress

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
C₄H_F₉	1H-Nonafluorobutane HCF ₂ CF ₂ CF ₂ CF ₃	J. Montgomery ¹ H. H. Michels ¹ J. Fournier ² S. Cooke ⁴	3 Conformers, assigned
C₅H₆O	2-Pentynal (Ethyl formyl acetylene) CH ₃ CH ₂ C≡CC(=O)H	R. Bohn J. Montgomery ¹	Heavy Atom Planar, 1 Conformer, assigned
C₆H₇N	5-Hexynenitrile HC≡CCH ₂ CH ₂ CH ₂ C≡N	K. Utzat A. Restrepo ⁵	4 conformers, assigned
C₆H₈O	3-Hexyne-2-one (Ethyl acetyl acetylene) CH ₃ CH ₂ C≡CC(=O)CH ₃	S. Stephens ³	Assigned, CH ₃ internal rotation splittings
C₆H₁₄	n-Hexane CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	R. Bohn	TTG conformer assigned
C₇H₁₀	2-Methyl-1-hexene-3-yne (Ethyl-2-propenyl acetylene) CH ₃ CH ₂ C≡CC(=CH ₂)CH ₃	J. Fournier ² S. Stephens ³	Assigned, CH ₃ internal rotation splittings
C₈H₁₀	3,5-octadiyne (Diethyl diacetylene) CH ₃ CH ₂ C≡C-C≡CCH ₂ CH ₃	J. Fournier ²	Assignment ambiguous Very low barrier
C₉H₆O	3-Phenyl Propynal (Phenyl formyl acetylene) C ₆ H ₅ C≡CCHO	R. Bohn	Heavy atom planar assigned, Tunneling
C₁₀H₁₀	1-Phenyl-1-butyne (Phenyl ethyl acetylene) C ₆ H ₅ C≡CCH ₂ CH ₃	R. Bohn	Tunneling. Qualitative assignment

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C₁₁H₁₂	1-Phenyl-3-methyl-1-butyne (1-Phenyl-2-propyl acetylene) C ₆ H ₅ C≡CCH(CH ₃) ₂	R. Bohn	Tunneling. 2 states. Qualitative assignment.

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Formula	Name of Compound	Name of Investigator	Present Stage of Progress
C ₅ H ₃ ClFN	2-chloro-3-fluoropyridine	Arnold, Chewning, Brown	spectrum assigned
C ₅ H ₃ ClFN	2-chloro-6-fluoropyridine	Arnold, Chewning, Brown	spectrum assigned
C ₆ H ₄ FNO ₂	2-fluoropyridine – CO ₂ complex	Brown, Hall, McCarthy(Harvard)	spectrum assigned
C ₆ H ₄ FNO ₂	3-fluoropyridine – CO ₂ complex	Brown, Parks, McCarthy(Harvard)	spectrum assigned
C ₅ H ₄ IN	3-iodopyridine	Gaster, Hall, Brown	spectrum assigned
C ₇ H ₄ F ₂ O (C ₆ H ₃ F ₂ COH)	2,3-difluorobenzaldehyde	Gaster, Parks, Brown	1 conformer assigned
C ₇ H ₄ F ₂ O (C ₆ H ₃ F ₂ COH)	2,6-difluorobenzaldehyde	Gaster, Parks, Brown	spectrum assigned
C ₇ H ₄ F ₂ O (C ₆ H ₃ F ₂ COH)	3,4-difluorobenzaldehyde	Brown, Gaster, McCarthy(Harvard)	<i>JCP</i> , 144 , (2016) 124201
C ₇ H ₄ F ₂ O (C ₆ H ₃ F ₂ COH)	3,5-difluorobenzaldehyde	Gaster, Parks, Yarbrough, Brown	1 conformer assigned
C ₆ H ₃ F ₂ NO ₂	2,3-difluoropyridine – CO ₂ complex	Gaster, Funderburk, Brown	spectrum assigned

Formula	Name of Compound	Name of Investigator	Present Stage of Progress
$C_{10}H_{12}O_2$	eugenol	Funderburk, Gaster, Brown, Shipman (NCF)	<i>JPC</i> , 123 (2019) 1091-1099.

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FORMULA	NAME OF COMPOUND	INVESTIGATORS	PRESENT STAGE OF PROGRESS
^{15}NH	imidogen	L. Bizzocchi, M. Melosso ¹ , L. Dore ¹ F. Tamassia ² , et al.	<i>ApJ</i> 863 , 3 (2018)
CH_2S_2	dithioformic acid	D. Prudenzano, et al.	<i>A&A</i> 612 , A56 (2018)
C_3HN	cyanoacetylene	L. Bizzocchi, M. Melosso ¹ , F. Tamassia ² , O. Pirali ³ , M.A.-Martin Drumel ³ H.S.P. Müller ⁴ , et al.	Higher excited states IR/submm-wave ongoing
C_3DN	<i>d</i> -cyanoacetylene	L. Bizzocchi, M. Melosso ¹ , L. Dore ¹ F. Tamassia ² , A. Pietropolli-Charmet ⁵ , et al.	IR/submm-wave manuscript in preparation
CHOS^+ CHOS^+	protonated carbonyl sulfide	V. Lattanzi, S. Spezzano, M. McCarthy ⁶ , et al.	<i>A&A</i> 620 , A184 (2018)
CD_2S	thioformaldehyde- <i>d</i> ₂	V. Lattanzi et al.	mm-wave and submm-wave measurements completed
CHS_2^+	protonated carbon disulfide	V. Lattanzi, M.E. Palumbo ⁷ , M. McCarthy ⁶ , et al.	measurements ongoing
C_2HO C_2DO	ketenyl <i>d</i> -ketenyl	J. Chantzios, S. Spezzano, et al.	<i>A&A</i> 621 , A111 (2019)
$\text{C}_2\text{H}_4\text{N}_2$	<i>N</i> -cyano-methylamine	D. Prudenzano, J.-C. Guillemin ⁸ , M. Carvajal-Zaera ⁹ , et al.	measurements ongoing
CN^+	cyanogen cation	V. Lattanzi, M. McCarthy ⁶ , et al.	measurements ongoing

FORMULA	NAME OF COMPOUND	INVESTIGATORS	PRESENT STAGE OF PROGRESS
NDH	amidogen	L. Bizzocchi, M. Melosso ¹ , L. Dore ¹ , O. Pirali ³ , M.A.-Martin Drumel ³ , et al.	manuscript in preparation
¹⁵ NDH	¹⁵ N-amidogen	L. Bizzocchi, M. Melosso ¹ , L. Dore ¹ , O. Pirali ³ , M.A.-Martin Drumel ³ , et al.	measurements ongoing
C ₃ H ₃ N	Propargyl-imine	D. Prudenzano, J.-C. Guillemin ⁸ et al.	E,Z isomers measurements ongoing
C ₂ H ₄ N	Allyl-imine	D. Prudenzano, A. Pietropolli-Charmet ⁵ , et al.	E,Z isomers measurements ongoing
CH ¹⁸ O ⁺ , CH ¹⁷ O ⁺	^{17,18} O-carbonylium	L. Bizzocchi, et al.	THz measurements completed manuscript in preparation
ArH ⁺	Argonium	L. Bizzocchi, M. Melosso ¹ , et al.	Ar broadening THz measurements in progress
C ₄ H ₅ N	Cyclopropyl cyanide	L. Bizzocchi, M. Melosso ¹ , A. Pietropolli-Charmet ⁵ , et al.	FIR spectrum analysis ongoing
C ₃ H ₄ N ₂	Imidazole	B.M. Giuliano, L. Bizzocchi, A. Steber ¹⁰ , M. Schnell ¹⁰ , et al.	Mm measurements completed manuscript in preparation

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
CH ₉ ClF ₃ NO [CClF ₃ ···N(CH ₃) ₃]	trifluorochloromethane···trimethylammonia	Caminati's group ⁱ Cocinero's group	Analysis in progress
C ₂ Cl ₃ F ₃ [CF ₃ CCl ₃]	CFC 113a	Kisiel ⁱⁱ Pszczółkowski ⁱⁱ Białkowska-Jaworska ⁱⁱ Jaworski ⁱⁱ Uriarte Basterretxea Cocinero	J. Mol. Spectr. <u>352</u> 1–9 (2018)
C ₂ Cl ₄ F ₂ [CCl ₂ FCCl ₂ F]	CFC 112a	Cocinero's group Kisiel's group ⁱⁱ	1 conformer assigned
C ₂ H ₆ F ₂ O ₂ [(C ₂ H ₂ F ₂)···(H ₂ O) ₂]	(Difluoromethane)···(Water) ₂	Cocinero's group Melandri's group ⁱ Pate's group ⁱⁱⁱ	submitted
C ₂ H ₈ F ₂ O ₃ [(C ₂ H ₂ F ₂)···(H ₂ O) ₃]	(Difluoromethane)···(Water) ₃	Cocinero's group Melandri's group ⁱ Pate's group	submitted
C ₄ H ₆ F ₄ O [(C ₂ H ₂ F ₂) ₂ ···(H ₂ O)]	(Difluoromethane) ₂ ···(Water)	Cocinero's group Melandri's group ⁱ Pate's group ⁱⁱⁱ	submitted
C ₄ H ₈ F ₄ O ₂ [(C ₂ H ₂ F ₂) ₂ ···(H ₂ O) ₂]	(Difluoromethane) ₂ ···(Water) ₂	Cocinero's group Melandri's group ⁱ Pate's group ⁱⁱⁱ	submitted
C ₁₀ H ₁₀ F ₁₀ [(C ₂ H ₂ F ₂) ₅]	(Difluoromethane) ₅	Cocinero's group Melandri's group ⁱ Pate's group ⁱⁱⁱ	1 complex assigned
C ₁₂ H ₁₂ F ₁₂ [(C ₂ H ₂ F ₂) ₆]	(Difluoromethane) ₆	Cocinero's group Melandri's group ⁱ Pate's group ⁱⁱⁱ	2 complexes assigned
C ₁₄ H ₁₄ F ₁₄ [(C ₂ H ₂ F ₂) ₇]	(Difluoromethane) ₇	Cocinero's group Melandri's group ⁱ Pate's group ⁱⁱⁱ	1 complex assigned
C ₃ H ₄ Cl ₂ F ₂ O [CHCl ₂ CF ₂ OCH ₃]	Methoxyflurane	Lesarri's group ^{iv} Cocinero's group Grabow's group ^v	Analysis in progress
C ₄ H ₈ O ₄	Erythrulose	Cocinero's group	1 conformer assigned

C ₆ H ₅ ClF ₃ N [C ₅ H ₅ N⋯CF ₃ Cl]	Pyridine⋯chlorotrifluoromethane	Gou ⁶ Vallejo-López Spada ¹ Staffolani ⁱ Lesarri ^{iv} Cocinero Caminati ⁱ	<i>Phys. Chem. Chem. Phys.</i> , <u>21</u> , 3545-3549 (2019)
C ₅ H ₁₃ NO ₂	2-aminopentano-1,3-diol	Cocinero's group Lesarri's group ^{iv}	In preparation
C ₆ H ₆ N ₂ O [C ₅ NH ₄ CONH ₂]	Nicotinamide	Caminati's group ⁱ Cocinero's group Lesarri's group ^{iv}	In preparation
C ₆ H ₁₀ O ₅	Levoglucofan	Uriarte Écija Lozada-García ⁷ Çarçabal ⁷ Cocinero	<i>ChemPhysChem.</i> , <u>19</u> , 766-773 (2018)
C ₆ H ₁₂ O	Oxacycloheptene	Lesarri's group ^{iv} Grabow's group ^v Cocinero's group	In preparation
C ₆ H ₁₂ O ₄ [CH ₂ (OH)CH ₂ (CHOH) ₂ COCH ₃]	Methyl- α -2-deoxyribofuranoside	Cocinero's group	submitted
C ₆ H ₁₂ O ₄ [CH ₂ (OH)CH ₂ (CHOH) ₂ COCH ₃]	Methyl- β -2-deoxyribofuranoside	Cocinero's group	submitted
C ₆ H ₁₂ O ₄ [CH ₂ (OH)CH ₂ (CHOH) ₂ COCH ₃]	Methyl- α -2-deoxyribofuranoside	Cocinero's group	submitted
C ₆ H ₁₂ O ₄ [CH ₂ (OH)CH ₂ (CHOH) ₂ COCH ₃]	Methyl- β -2-deoxyribofuranoside	Cocinero's group	submitted
C ₆ H ₁₁ FO ₅	2-fluoro-2-deoxyglucose	Cocinero's group	2 conformers assigned
C ₆ H ₁₂ O ₅	2-deoxyglucose	Cocinero's group	3 conformers assigned
C ₆ H ₁₂ O ₅	2-deoxygalactose	Cocinero's group	1 conformer assigned
C ₆ H ₁₁ FO ₅	2-fluoro-2-deoxymannose	Cocinero's group	2 conformers assigned
C ₇ H ₆ N ₂	Indazole	Cocinero's group	submitted
C ₁₀ H ₁₀ O ₂ [C ₆ H ₅ CHCHCOOCH ₃]	Methyl cinnamate	Cocinero's group Lesarri's group ^{iv}	2 conformers assigned
C ₁₀ H ₁₂ O ₃ [HOC ₆ H ₃ (OCH ₃)CHCHCH ₂ OH]	Coniferyl alcohol	Cocinero's group Lesarri's group ^{iv}	In preparation
C ₁₀ H ₁₄ O ₃ [HOC ₆ H ₃ CH ₂ CH ₂ CH(CO)CH ₃]	Zingerone	Uriarte Insausti Cocinero Jabri ⁸ Kleiner ⁸ Mouhib ⁸ Alkorta ⁹	<i>J. Phys. Chem. Lett.</i> , <u>9</u> , 5906–5914 (2018)
C ₁₁ H ₁₅ NO ₂ [NH ₂ C ₆ H ₄ COO(CH ₂) ₃ CH ₃]	Butamben	Lesarri's group ^{iv} Caminati's group ⁱ Cocinero's group Grabow's group ^v	Submitted
C ₁₁ H ₁₅ NO ₂ [NH ₂ C ₆ H ₄ COOCH ₂ CH(CH ₃) ₂]	Isobutamben	Lesarri's group ^{iv} Cocinero's group	Submitted
C ₁₂ H ₂₂ O ₂	Oxacyclotridecan-2-one	Cocinero's group Melandri's group ⁱ	2 conformer assigned
C ₁₃ H ₂₀ O	α -ionone	Cocinero's group Melandri's group ⁱ	<i>J. Phys. Chem. Lett.</i> , <u>9</u> , 1497-1502 (2018)
C ₁₃ H ₂₀ O	β -ionone	Cocinero's group Melandri's group ⁱ	<i>J. Phys. Chem. Lett.</i> , <u>9</u> , 1497-1502 (2018)
C ₁₃ H ₂₀ O	β -damascone	Cocinero's group Melandri's group ⁱ	<i>J. Phys. Chem. Lett.</i> , <u>9</u> , 1497-1502 (2018)

$C_{13}H_{20}O_3$	Methyl-jasmonate	Uriarte Insausti Cocinero Jabri ⁸ Kleiner ⁸ Mouhib ⁸ Alkorta ⁹	J. Phys. Chem. Lett. , <i>9</i> , 5906–5914 (2018)
$C_{15}H_{12}O_2$ [$C_6H_5COCH_2COC_6H_5$]	Dibenzoylmethane	Cocinero's group Caminati's group ⁱ	1 conformer observed

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
O ₃ U	Uranium (VI) oxide	B. E. Long [†]	Spectrum observed.
O ₂ Th	Thorium (IV) oxide	B. E. Long [†]	Spectrum observed.
C ₅ H ₂ F ₈	Cis-1H,2H-Perfluorocyclopentane	A. J. Minei [□]	Parent and minor isotopologues observed and assigned. Manuscript in prep
C ₅ H ₃ F ₇	1H,1H,2H-Perfluorocyclopentane	A. J. Minei [□]	Parent and minor isotopologues observed and assigned. Manuscript in prep
C ₄ HF ₉	2H-Nonafluorobutane		Parent and minor isotopologues observed and assigned
C ₅ Cl ₂ F ₆	1,2-dichlorohexafluorocyclopentene-1		Spectrum assigned
C ₆ Cl ₂ F ₈	1,2-dichlorooctafluorocyclohexene-1		Spectrum assigned
C ₃ F ₅ ClO	Chloropentafluoro acetone	W. C. Bailey ^Δ	Manuscript in preparation
C ₃ F ₄ Cl ₂ O	1,3-Dichlorotetrafluoro acetone		Manuscript in preparation

$C_3H_2F_3ClO$	1,1,1-Trifluoro-3-chloroacetone		Manuscript in preparation
$C_3H_4F_2O$	1,1-Difluoroacetone	P. Groner [≡] L. Margulès, R. Motiyenko [§]	CP-FTMW Spectrum Assigned mmW spectrum recorded.
C_3H_5ClO	Chloroacetone	B. E. Long [⊥]	Spectrum assigned
C_3F_5N	Perfluoropropionitrile	B. E. long [⊥]	Spectrum Assigned
BaS	Barium Monosulfide	G. S. Grubbs II [•]	Hyperfine structure, J = 1 - 0, 2 - 1 in high vibrational states.
C_3F_6NH	Hexafluoroacetone imine	G. S. Grubbs II [•] , D. Obenchain [⊥] , D. Frohman, S. E. Novick [⊥] , W. C. Pringle [⊥]	Spectrum assigned
C_4F_9I	Perfluoroiodobutane	G. S. Grubbs II [•] , R. Bohn	Manuscript in preparation
$C_4F_3H_6I$	3-Iodo-1,1,1-trifluorobutane	W. C. Bailey ^Δ	CP-FTMW spectrum assigned
C_3F_7HO	1,2,2,2-Tetrafluoroethyl trifluoromethyl ether	A. Turk	Spectrum assigned
$C_5F_7H_3O_2$	2,2,3,3-Tetrafluoropropyl trifluoroacetate		Spectrum assigned
$C_4H_7ClF_2O$	1-chloro-1,1-difluoro-2-methyl-2-propanol		Spectrum assigned
$C_3H_4F_3I$	1,1,1-trifluoro-3-iodopropane	W. C. Bailey ^Δ	Manuscript in preparation
$C_3H_2F_5I$	1,1,1,2,2-pentafluoro-3-iodopropane	W. C. Bailey ^Δ	Manuscript in preparation
$C_{10}F_{19}N$	Perfluorodecanonitrile	A. J. Minei [□]	Spectrum observed

$C_3H_6F_3N$	1,1,1-Trifluoro-3-azapent-3-ene	C. T. Dewberry	Spectrum assigned
$C_5H_{11}F$	1-Fluoropentane	D. Obenchain [†]	Spectrum Assigned
$C_6H_{13}F$	1-Fluorohexane	D. Obenchain [‡]	Spectrum Assigned
$C_7H_{15}F$	1-Fluoroheptane	D. Obenchain [‡]	Spectrum Assigned
$C_8H_{17}F$	1-Fluorooctane	D. Obenchain [‡] , W. Orellana [‡]	Spectrum Assigned
$C_5H_{12}S$	Butyl methyl thioether	J. Ogulnick, T. Holmes	Spectrum Assigned
$C_6H_{14}S$	Pentyl methyl thioether	J. Ogulnick, T. Holmes	Spectrum Assigned
$C_3H_5F_5S$	Propene-1-yl pentafluorosulfur	W. Orrellana [‡] , S. Stephens [‡] , S. Novick [‡]	4-fold internal rotor problem analyzed. Manuscript in preparation.
$C_4H_7F_5S$	Butene-1-yl pentafluorosulfur	W. Orrellana [‡] , S. Stephens [‡] , S. Novick [‡]	4-fold internal rotor problem analyzed. Manuscript in preparation.

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR(S)	PRESENT STATE OF PROGRESS
BF ₂ HO (BF ₂ OH)	Hydroxydifluoroborane	Drouin, Fry	mm and submm spectra recorded, analyzed
CCl ₂ O (COCl ₂)	Carbonyl chloride (phosgene)	Drouin	Millimeter wave spectra analyzed, spectra for mixed isotopomer
CH ₃ DO (CH ₂ DOH)	Deuterated Methanol	Pearson, Yu, & Drouin	Ext. J,K analysis in progress
CH ⁺	Methylidyne	Yu, Amano, Pearson, & Drouin	Isotopic and main species data up to 2.5 THz, published ¹
CHN (HCN)	Hydrogen cyanide	Pearson, Yu, & J. Cernicharo	Vib. Excited rotational data recorded, analyzed
CH ₃ NO ₃	Methyl nitrate	Drouin, & Xhang	Submm data acquired, assigned
CH ₄	Methane	Drouin	2.5-2.7 THz spectra for ¹² C, ¹³ C
C ₅ H ₈	Isoprene	Drouin, Kisiel, Porterfield, & Martin	100-300 GHz spectra collected, analysis in progress
ClH (HCl)	Hydrogen Chloride	Gupta, Drouin, & Pearson	THz spectra to v=8
ClO	Chlorine Monoxide	Cohen, Drouin, & L. Duffy (UNC Greensboro)	Rotational data to v=8, analysis complete
CH ₂ ⁺ (H ₂ Cl ⁺)	Chloronium	Gupta, Drouin, & Pearson	THz spectra recorded
CO ₂	Carbon Dioxide (¹⁸ OCO)	Drouin, & B. Elliot	Isotopic measurements 0.5-0.6 THz
C ₂ HD (HCCD)	Deuterated Acetylene	Yu, Drouin, & A. Walters (CESR)	THz spectra measured, assigned
C ₃ H ₅ N (CH ₃ CH ₂ CN)	Propionitrile (ethyl cyanide)	Pearson, Daly, Alonzo (U Vallalodid), & Yu	Excited vibrational analyses in progress
H ¹⁵ NO ₂	Nitrous Acid	Drouin & Miller	Submillimeter spectra recorded, assigned
HO ₂	Hydroperoxyl radical	Drouin	N ₂ and O ₂ temperature dependent pressure broadening
H ₂ O	Water (¹⁷ O & ¹⁸ O)	Yu, Drouin, Pearson, & Walters (CNRS)	Measurements through 2.6 THz for ¹⁸ O and 2.7THz for ¹⁷ O
H ₂ N	Amidogen	Müller (Köln) & Drouin	Gs analysis complete, excited vibrational state analysis in progress

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR(S)	PRESENT STATE OF PROGRESS
H ₃ N	Ammonium	Pearson, Yu, Sung, Drouin, & Pirali	Hamiltonian model for 3v ₂ and v ₄ +v ₂ , published ²
O ₂ S (SO ₂)	Sulfur Dioxide	Drouin	Temperature dependent air pressure broadening

¹J. Pearson, S. Yu, J. Pearson, K. Sung, B. Drouin, O. Pirali, "Extended measurements and an experimental accuracy effective Hamiltonian model for the 3 v₂ and v₄+ v₂ states of ammonia", J. Mol. Spec. 353, 60, 2018.

²S. Yu, B.J. Drouin, J.C. Pearson and T. Amano, "THz Spectroscopy of ¹²CH⁺, ¹³CH⁺, and ¹²CD⁺: A combined Dunham analysis of Terahertz lines and A1\Pi- X1\Sigma⁺ transitions", J. Mol. Spec. 350, 30, 2018.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
H ₄ O ₂ (H ₂ O-H ₂ O)	water dimer	W. Caminati et al.	High J, high K transitions observed
CClF ₃ Kr (CCl ₃ -Kr)	chlorotrifluoromethane krypton	L. Evangelisti	Asymmetric top spectrum
CH ₂ ClFNe (CH ₂ ClF-Ne)	chlorofluoromethane neon	P. Ottaviani et al. ISMN	Spectrum observed, dynamics
CH ₂ F ₂ Ne (CH ₂ F ₂ -Ne)	difluoromethane neon	S. Melandri et al.	Spectrum assigned, dynamics
CH ₃ F ₄ N (CF ₄ -NH ₃)	tetrafluoromethane ammonia	L. Evangelisti et al.	Symmetric top, tunneling
CH ₄ F ₃ N (CHF ₃ -H ₃ N)	trifluoromethane ammonia	B.M. Giuliano et al.	mmw measurements
CH ₆ O ₂ (CH ₃ OH-H ₂ O)	methanol water	S. Melandri et al.	High J, high K transitions observed
C ₂ F ₄ O (CF ₄ -CO)	tetrafluoromethane carbon monoxide	L. Evangelisti et al.	Spectrum assigned, symmetric top
C ₂ F ₃ KrN (C ₂ F ₃ N-Kr)	trifluoroacetonitrile krypton	L. Evangelisti et al.	Symmetric top
C ₂ H ₂ F ₄ O (C ₂ F ₄ -H ₂ O)	tetrafluoroethene water	Q. Gou et al. CQU	Spectrum recorded
C ₂ H ₃ F ₃ Cl ₂ (CH ₃ Cl-CF ₃ Cl)	chloromethane chlorotrifluoromethane	W. Li et al.	Spectrum assigned
C ₂ H ₃ F ₃ O (CHF ₃ -CH ₂ O)	trifluoromethane formaldehyde	Q. Gou et al. UVA, UPV, CQU	1 conformer, 4 states
C ₂ H ₄ NeO (C ₂ H ₄ O-Ne)	oxirane neon	S. Melandri et al. PhLAM	Spectrum assigned, dynamics

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_2H_6Cl_2Ge$	dichlorodimethylgermane	P. Ottaviani et al. PCI	Internal rotation, quadrupole
$C_2H_6Cl_2Sn$	dichlorodimethylstannane	P. Ottaviani et al. PCI	Spectrum assigned
C_2H_7ClO (C_2H_6O-HCl)	dimethylether hydrogen chloride	W. Caminati et al. UVA, SU	Hyperfine structure
$C_2H_7NO_3$ ($C_2H_5NO_2-H_2O$)	glycolamide water	A. Maris et al.	Spectrum assigned
$C_2H_8N_2O_2$ ($C_2H_5NO_2-H_3N$)	glycolamide ammonia	A. Maris et al.	Spectrum assigned
$C_2H_8O_2$ ($C_2H_6O-H_2O$)	dimethylether water	W. Caminati et al. SU	Manuscript in preparation
$C_2H_8O_2$ (CH_4O-CH_4O)	Methanol Dimer	S. Melandri et al.	High J, high K transitions observed
C_3ClF_7 ($C_2F_4-CClF_3$)	tetrafluoroethene chlorotrifluoromethane	G. Feng et al. CQU	Spectrum recorded
C_3F_3NO (C_2F_3N-CO)	trifluoroacetonitrile carbon monoxide	L. Evangelisti et al.	Symmetric top
$C_3H_4O_2$	acrylic acid	C. Calabrese et al. UBO	Submm-wave spectrum, excited states
$C_3H_4F_4O_2$ ($CF_4-C_2H_4O_2$)	tetrafluoromethane ethylene oxide	G. Feng et al. CQU	Manuscript submitted
C_3H_5N	Propargylamine	M. Melosso et al. UBO	Isotopologues assigned
$C_3H_5NO_2$	1,3-oxazolidin-2-one	A. Maris et al.	Spectrum assigned, tunnelling
$C_3H_6N_2O$	ethylene urea	A. Vigorito et al.	Spectrum assigned, tunneling
$C_3H_6F_4O$ ($C_2H_6O-CF_4$)	Dimethylether Tetrafluoromethane	L. Evangelisti et al. ISMN	1 conformer, 4 states
$C_3H_6O_2$	1,3-dioxolane	A. Maris et al. UBO	Splittings in various states
$C_3H_6O_2$ ($C_2H_4O-H_2O$)	Acroleine Water	W. Li et al.	Manuscript ready
$C_3H_6O_3$ ($C_3H_4O_2-H_2O$)	acrylic acid water	A. Maris et al. ISMN	2 conformers, 9 isotopologues
$C_3H_7F_3O$ ($C_2H_6O-CHF_3$)	dimethylether trifluoromethane	W. Caminati et al. EIU	H-bond, dynamics

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₃ H ₇ NO ₃ (C ₃ H ₅ NO ₂ -H ₂ O)	1,3-oxazolidin-2-one Water	A. Maris et al.	Spectrum assigned, tunnelling
C ₃ H ₈ N ₂ O ₂ (C ₃ H ₆ N ₂ O-H ₂ O)	Ethyleneurea Water	A. Maris et al.	Spectrum assigned
C ₄ H ₄ O ₄ (C ₃ H ₄ O ₂ -CO ₂)	acrylic acid carbon dioxide	A. Maris	2 conformers assigned
C ₄ H ₄ F ₄ O ₄	<i>alpha, alpha</i> -difluoroacetic acid dimer	Q. Gou et al. CQU	4 states, proton tunneling
C ₄ H ₆ O ₄ (C ₂ H ₄ O ₂ -CH ₂ O ₂)	<i>beta</i> -propiolactone formic acid	L. Evangelisti et al. UVA	Spectrum assigned
C ₄ H ₆ F ₄ O (C ₂ H ₆ O-C ₂ F ₄)	dimethylether tetrafluoroethene	L. Evangelisti et al.	Spectrum recorded
C ₄ H ₇ NO	2-pyrrolidinone	A. Maris et al.	Spectrum assigned, ND species
C ₄ H ₇ NO (C ₃ H ₃ N-CH ₄ O)	acrylonitrile methanol	C. Calabrese et al.	Manuscript in preparation
C ₄ H ₇ NO ₂	3-methyl-1,3-oxazolidin-2- one	A. Maris et al.	Spectrum assigned, tunnelling, V ₃
C ₄ H ₈ O	1-methylcyclopropanol	W. Li et al.	Spectrum assigned, tunneling
C ₄ H ₈ O ₂	isopropylformate	L. Spada et al. ISMN	Spectrum assigned
C ₄ H ₉ NO ₂ (C ₄ H ₇ NO-H ₂ O)	2-pyrrolidinone Water	A. Maris et al.	Spectrum assigned, ND species
C ₄ H ₁₂ O ₄ (C ₆ H ₁₈ O ₆)	Ethylene glycol dimer (and trimer)	Usabiaga et al. UVA	Spectrum assigned
C ₄ D ₈ O	tetrahydrofuran- <i>d</i> ₈	A. Maris et al. UVA, RM	Pseudorotation splittings
C ₄ H ₉ ClF ₃ N (CClF ₃ -C ₃ H ₉ N)	chlorotrifluoromethane trimethylamine	L. Evangelisti et al. UPV	Halogen bond
C ₄ H ₁₀ N ₂ O ₄ (C ₂ H ₅ NO ₂) ₂	Nitroethane dimer	W. Li et al.	Spectrum recorded
C ₄ H ₁₀ O ₂	1,2-butanediol	A. Vigorito et al.	6 conformers, OD & ¹³ C species
C ₄ H ₁₀ O ₃	trimethoxymethane	G. Feng et al. LISA	3 conformers assigned
C ₄ H ₁₀ S ₂	1,4-butanedithiol	A. Vigorito et al.	4 conformers assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₅ H ₃ F ₄ NO (C ₅ HF ₄ N-H ₂ O)	2,3,4,6-trifluoropyridine Water	C. Calabrese et al.	Spectrum assigned, MS in prep.
C ₅ H ₄ F ₃ NO (C ₅ H ₂ F ₃ N-H ₂ O)	2,4,6-trifluoropyridine Water	C. Calabrese et al.	Spectrum assigned, MS in prep.
C ₅ H ₅ F ₂ NO (C ₅ H ₃ F ₂ N-H ₂ O)	3,5-difluoropyridine Water	C. Calabrese et al.	Spectrum assigned, MS in prep.
C ₅ H ₅ F ₂ NO (C ₅ H ₃ F ₂ N-H ₂ O)	2,6-difluoropyridine Water	C. Calabrese et al.	Spectrum assigned, MS in prep.
C ₅ H ₈ O ₂	acetylacetone	W. Caminati et al. PCI, KU	Spectrum observed
C ₅ H ₁₀ O ₃ (C ₄ H ₈ O-CH ₂ O ₂) (C ₄ H ₈ O-CHDO ₂)	1-methylcyclopropanol formic acid	W. Li et al.	Spectrum assigned
C ₅ H ₁₂ O	2-methyl-2-butanol	L. Spada et al. ISMN	5 conformers assigned
C ₅ H ₁₂ O ₃ (CH ₂ O ₂ -C ₄ H ₁₀ O)	formic acid <i>tert</i> -butanol	L. Evangelisti et al.	Spectrum assigned, tunneling
C ₆ F ₅ NO (C ₅ F ₅ N-CO)	Pentafluoropyridine CO	S. Melandri et al.	Spectrum assigned
C ₆ H ₃ F ₂ N (C ₅ F ₅ N-CFH ₃)	Pentafluoropyridine fluoromethane	S. Melandri et al.	Spectrum assigned
C ₆ H ₃ F ₆ N (C ₆ F ₆ -NH ₃) (C ₆ F ₆ - ¹⁵ NH ₃)	hexafluorobenzene ammonia	S. Melandri et al. ISMN	Spectrum assigned
C ₆ H ₅ ClF ₃ N (C ₅ H ₅ N-CClF ₃)	pyridine chlorotrifluoromethane	Q. Gou et al. CQU	Halogen bond
C ₆ H ₇ NO ₂ S	benzenesulfonamide	S. Melandri et al. KCL	Spectrum assigned, ND species
C ₆ H ₈ N ₂ O ₂ S	sulfanilamide	A. Vigorito et al. KCL	Spectrum assigned
C ₆ H ₉ NO (C ₅ H ₅ N-CH ₄ O)	pyridine methanol	L. Evangelisti et al.	Spectrum assigned
C ₆ H ₁₀ N ₂ (C ₃ H ₅ N-C ₃ H ₅ N)	propargylamine dimer	L. Spada et al. UBO	Spectrum assigned
C ₆ H ₁₂ F ₃ N (C ₅ H ₁₁ N-CHF ₃)	<i>N</i> -methylpyrrolidine trifluoromethane	L. Evangelisti et al.	H-bond, internal rotation
C ₆ H ₁₂ O	<i>cyclo</i> -hexanol	W. Li et al. UVA	2 conformers assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₁₂ O ₂	<i>trans</i> -1,2-cyclohexanediol	W. Caminati et al.	Spectrum assigned, OD species
C ₆ H ₁₄ O ₃ (C ₂ H ₆ O-C ₄ H ₈ O ₂)	ethanol 1,4-dioxane	L. Evangelisti et al.	1 conformer observed
C ₇ F ₆ O (C ₆ F ₆ -CO)	hexafluorobenzene carbon monoxide	S. Melandri et al. ISMN	Spectrum assigned
C ₇ H ₆ F ₂ O	2,6-difluorobenzylalcohol	L. Evangelisti et al.	Spectrum assigned, tunnelling
C ₇ H ₉ NO ₂ S	<i>p</i> -toluenesulfonamide	C. Calabrese et al. KCL	3 species assigned
C ₇ H ₉ NO ₂ S	<i>o</i> -toluenesulfonamide	A. Vigorito et al. KCL	Spectrum assigned, V ₃
C ₇ H ₁₁ NO (C ₇ H ₉ N-H ₂ O)	benzylamine water	S. Melandri et al.	1 conformer
C ₇ H ₁₂ O ₂	3,5-heptanedione	L. Evangelisti et al.	2 conformers
C ₇ H ₁₄ O ₃ (C ₇ H ₁₂ O ₂ -H ₂ O)	3,5-heptanedione Water	W. Li et al.	2 conformers
C ₇ H ₁₂ O ₂	<i>cyclo</i> -hexylformate	L. Evangelisti et al.	1 conformer
C ₈ H ₈ O	<i>p</i> -tolualdehyde	W. Caminati et al. PCI, LISA, NIST	V ₃ & V ₆
C ₈ H ₈ O ₂	phenyl acetate	W. Caminati et al.	Spectrum assigned
C ₈ H ₁₀ FN	<i>p</i> -fluorophenylethylamine	S. Melandri et al.	2 conformers assigned
C ₈ H ₁₆ O	1-octen-3-ol	A. Maris et al.	2 conformers assigned
C ₈ H ₁₈ N ₂ (C ₄ H ₉ N-C ₄ H ₉ N)	pyrrolidine dimer	A. Maris et al. ISMN	Spectrum assigned
C ₉ H ₉ F ₆ N (C ₆ F ₆ -N(CH ₃) ₃)	Hexafluorobenzene Trimetilamina	W. Li et al.	Spectrum assigned
C ₁₀ H ₁₂ O ₂	eugenol	A. Maris et al.	Spectrum assigned
C ₁₃ H ₁₃ F ₆ N (C ₆ F ₆ -C ₇ H ₁₃ N)	Hexafluorobenzene Quinuclidine	W. Li et al.	Spectrum assigned
CQU	Chongqing School of Chemistry and Chemical Engineering, Chongqing University (RPC)		
EIU	Department of Chemistry, Eastern Illinois University (USA)		
ISMN	Istituto per lo Studio dei Materiali Nanostrutturati, CNR Sezione di Bologna (I)		
KCL	King's College London (UK)		
KU	Department of Chemistry, University of Copenhagen (DK)		
LISA	Laboratoire Inter-Universitaire des Systemes Atmospheriques, Université Paris Est Creteil (F)		

NIST National Institute of Standards and Technology (USA)
PCI Institut für Physikalische Chemie & Elektrochemie, Universität Hannover (D)
PhLAM Laboratoire de Physique des Lasers, Atoms and Molecules, Villeneuve d'Ascq (F)
RM Rolf Meyer, Zefikon (CH)
SU Department of Chemistry, Shizuoka University (J)
UPV Departamento de Química Física, Universidad del País Vasco, Leioa (E)
UVA Departamento de Química Física, Universidad de Valladolid (E)
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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₅ H ₁₁ NO (HCONHC(CH ₃) ₃)	N-tert-Butylformamide	Masaharu Fujitake	Manuscript in prep. Z, E-form
C ₅ H ₁₃ NO ₂ (C ₅ H ₁₁ NO-H ₂ O)	N-tert-Butylformamide -water	Masaharu Fujitake	Manuscript in prep. Two conformers
C ₅ H ₁₅ NO ₃ (C ₅ H ₁₁ NO-H ₄ O ₂)	N-tert-Butylformamide -(water) ₂	Masaharu Fujitake	Manuscript in prep.
C ₆ H ₁₅ NO ₂ (C ₅ H ₁₁ NO-CH ₃ OH)	N-tert-Butylformamide -methanol	Masaharu Fujitake	Manuscript in prep. Two conformers
C ₆ H ₁₄ N ₂ O ₂ (C ₅ H ₁₁ NO-HCONH ₂)	N-tert-Butylformamide -formamide	Masaharu Fujitake	Spectrum assigned. formamide- ¹⁵ N
C ₄ H ₁₁ NO ₂ (C ₄ H ₉ NO-H ₂ O)	N,N-Dimethylacetamide -water	Masaharu Fujitake	Spectrum assigned. V ₃ of 3 methyl tops
C ₄ H ₁₀ O ₄ (C ₄ H ₈ O ₃ -H ₂ O)	Methyl lactate-water	Masaharu Fujitake	Manuscript in prep. Three conformers

Lab 11

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₁₂ O ₅ (C ₄ H ₈ O ₃ -(H ₂ O) ₂)	Methyl lactate-(water) ₂	Masaharu Fujitake	Spectrum assigned. Two conformers
C ₅ H ₁₂ O ₅ (C ₄ H ₈ O ₃ -CH ₃ OH)	Methyl lactate-methanol	Masaharu Fujitake	Spectrum assigned.
C ₃ H ₄ D ₃ NO (CH ₃ CONHCD ₃)	N-methylacetamide(NCD ₃)	Masaharu Fujitake	Spectrum assigned.
C ₃ H ₆ DNO (CH ₃ CONDCH ₃)	N-methylacetamide(ND)	Masaharu Fujitake	Spectrum assigned.
C ₃ H ₄ D ₃ NO (CD ₃ CONHCH ₃)	N-methylacetamide(CCD ₃)	Masaharu Fujitake	Spectrum assigned.
C ₃ H ₉ NO ₂ (C ₃ H ₇ NO-H ₂ O)	N-methylacetamide-water	Masaharu Fujitake	Spectrum assigned. Two conformers
C ₃ H ₆ D ₃ NO ₂ (CD ₃ CONHCH ₃ -H ₂ O)	N-methylacetamide(CCD ₃) -water	Masaharu Fujitake	Spectrum assigned.
C ₃ H ₆ D ₃ NO ₂ (CH ₃ CONHCD ₃ -H ₂ O)	N-methylacetamide(NCD ₃) -water	Masaharu Fujitake	Spectrum assigned.
C ₃ H ₉ NO ¹⁸ O (CH ₃ CONHCH ₃ -H ₂ ¹⁸ O)	N-methylacetamide -(H ₂ ¹⁸ O)water	Masaharu Fujitake	Spectrum assigned.
C ₃ H ₇ D ₂ NO ₂ (CH ₃ CONHCH ₃ -D ₂ O)	N-methylacetamide -(D ₂ O)water	Masaharu Fujitake	Spectrum assigned.
C ₃ H ₈ DNO ₂ (CH ₃ CONHCH ₃ -DOH)	N-methylacetamide -(DOH)water	Masaharu Fujitake	Spectrum assigned.

Lab 11

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_8DNO_2$ ($CH_3CONHCH_3-HOD$)	N-methylacetamide -(HOD)water	Masaharu Fujitake	Spectrum assigned.
$C_3H_{10}O_5$ ($C_3H_6O_3-(H_2O)_2$)	Methyl glycolate -(water) ₂	Masaharu Fujitake	Spectrum assigned.
$C_4H_{10}O_4$ ($C_3H_6O_3-CH_3OH$)	Methyl glycolate -methanol	Masaharu Fujitake	Spectrum assigned.
$C_4H_{11}NO$ ($NH_2CH_2C(CH_3)_2OH$)	1-Amino-2-methyl-2-propanol	Masaharu Fujitake	Spectrum assigned.
$C_4H_{13}NO_2$ ($NH_2CH_2C(CH_3)_2OH-H_2O$)	1-Amino-2-methyl-2-propanol -water	Masaharu Fujitake	Spectrum assigned. Two conformers
$C_4H_9NO_2$ ($HCONH_2-(CH_2)_3O$)	Formamide -trimethylene oxide	Masaharu Fujitake	Spectrum assigned.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₂ F ₄ O (C ₂ F ₄ -H ₂ O)	Tetrafluoroethylene-water complex	Qian Gou ¹	Spectrum recorded
C ₂ H ₂ F ₄ OS ₂ (C ₂ S ₂ F ₄ -H ₂ O)	Tetrafluoro-1,3-dithietane-water complex	Yan Jin	Manu. Submitted
C ₂ H ₃ Cl ₂ F ₃	CH ₃ Cl-CF ₃ Cl complex	Yang Zheng, Tao Lu, Luca Evangelisti ¹	Spectra recorded
C ₂ H ₃ F ₅ O (CF ₃ CF ₂ H-H ₂ O)	pentafluoroethane-water complex	Qian Gou, Gang Feng ^{1,2,3}	Manu. Ready
C ₂ H ₃ NO ₃ (HCONH ₂ -CO ₂)	formimade-CO ₂ complex	Shuang Gao, Daniel A. Obenchain ²	<i>Phys. Chem. Chem. Phys.</i> 2019 , DOI:10.1039/C9CP00055K
C ₂ H ₃ F ₃ O (CF ₃ H-CH ₂ O)	Trifluoromethane-formaldehyde complex	Qian Gou ^{1,3,4}	1 conformer, 4 states
C ₂ H ₃ F ₄ NS ₂ (C ₂ S ₂ F ₄ -NH ₃)	Tetrafluoro-1,3-dithietane-ammonia complex	Xiaolong Li	Manuscript in preparation; Spectra assigned, ³⁴ S, ¹³ C and ¹⁵ N isotopes, internal rotation
C ₂ H ₅ NS	Thioacetamide	Jiaqi Zhang	Spectra assigned, one conformer, internal rotation of -CH ₃
C ₂ H ₆ O ₂ S ₃ (CH ₃ S ₂ CH ₃ -SO ₂)	Dimethyl Disulfide-SO ₂ complex	Xiaolong Li	Spectra recorded, analysis in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_4F_6$ ($CH_2F_2-CFH_2CF_3$)	Difluoromethane–tetrafluoroethane complex	Tao Lu	Chemphyschem 19, 2655 (2018).
$C_3H_8F_2O$ ($CH_2FCH_2CH_2F-H_2O$)	1,3-difluoropropane-water complex	Tao Lu	J. Chem. Phys. 150, 064305 (2019).
C_3H_9N ($CH_3CH(NH_2)CH_3$)	isopropylamine	Junhua Chen, Lorenzo Spada ¹	Spectra assigned, two conformers,
C_3H_9N	n-Propylamine	Tao Lu, Yang Zheng, Lorenzo Spada ¹	Spectra assigned, four conformers
$C_3H_{11}NO$ ($CH_3CH(NH_2)CH_3-H_2O$)	isopropylamine-water complex	Junhua Chen, Lorenzo Spada ¹	Spectra assigned, two conformers, 3- $C^{13}, H_2O^{18}, D_2O, DOH, HOD$
$C_3H_{11}NO$ ($C_3H_9N-H_2O$)	n-Propylamine-water	Yang Zheng ¹	Spectra assigned, three conformers
$C_4H_2F_8O$ ($C_4F_8-H_2O$)	octafluorocyclobutane-water	Junhua Chen ^{1,3}	Spectra assigned, one conformer, O^{18}, D_2O, DOH , tunneling splitting, four states,
$C_4H_3F_8N$ ($C_4F_8-NH_3$)	octafluorocyclobutane-ammonia	Junhua Chen	Spectra assigned, one conformer, tunneling splitting
C_4H_3ClS (C_4SH_3Cl)	2-chlorothiophene	Yan Jin	Manu. Submitted
C_4H_3ArClS (C_4SH_3Cl-Ar)	2-chlorothiophene-Ar	Yan Jin	Manu. Submitted
$C_4H_4F_4O_4$ (CF_2HCOOH) ₂	α, α -F ₂ -acetic acid dimer	Qian Gou ¹	4 states, proton tunneling
$C_4H_8F_6$ ((CH_2F_2) ₂ - CH_3CHF_2)	(CH_2F_2) ₂ - CH_3CHF_2 trimer	Tao Lu	Spectra assigned, two conformers
$C_4H_8O_3$ ($CH_3OCOCH_2COCH_3$)	Methyl methoxyacetate	Juncheng Lei	Spectra assigned, one conformer, internal rotation of - CH_3
$C_4H_9O_2N$ ($CH_3CH(NH_2)CH_3-CO_2$)	isopropylamine-CO ₂ complex	Tao Lu, Jiaqi Zhang	Spectra assigned, two conformers
$C_4H_{10}ArS_2$ ($CH_3CH_2S_2CH_2CH_3-Ar$)	diethyl disulfide-Ar complex	Gang Feng ²	Spectra assigned, one conformer

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₁₀ O ₃ (CH(OCH ₃) ₃)	trimethoxymethane	Gang Feng ^{1,5}	3 conformers assigned
C ₄ H ₁₂ OS (CH ₃ CH ₂ OH- CH ₃ CH ₂ SH)	ethanol-ethanethiol	Yan Jin, Jiaqi Zhang, Xiaolong Li ³	Spectrum Assigned, one conformer
C ₄ H ₁₂ S ₂ (CH ₃ CH ₂ SH- CH ₃ CH ₂ SH)	ethanethiol-ethanethiol	Jiaqi Zhang, Xiaolong Li ³	Spectrum Assigned, one conformer, tunneling splitting
C ₄ H ₁₂ OS ₂ (CH ₃ CH ₂ S ₂ CH ₂ CH ₃ - H ₂ O)	diethyl disulfide-water complex	Xiaolong Li, Jes- Uwe Grabow ²	Spectra assigned, one conformer, O ¹⁸ , D ₂ O, DOH, HOD tunneling splitting
C ₅ HF ₄ N (2,3,4,6-FC ₅ H)	2,3,4,6-Tetrafluoropyridine	Juan Wang	spectra assigned, ¹³ C and ¹⁵ N isotopologues
C ₅ H ₄ F ₃ NO (C ₅ H ₂ F ₃ N-H ₂ O)	2,3,6-Trifluoropyridine-water complex	Juan Wang ¹	Manuscript in preparation, ¹⁸ O, D ₂ O, DOH, HOD isotopes
C ₅ H ₄ O ₃ (C ₄ H ₄ O-CO ₂)	furan-CO ₂	Juncheng Lei	Spectra assigned, one conformer,
C ₅ H ₅ F ₂ NO (C ₅ H ₃ F ₂ N-H ₂ O)	2,3-difluoropyridine-water complex	Juan Wang ¹	Manuscript in preparation ¹⁸ O, D ₂ O, DOH, HOD isotopes
C ₅ H ₅ F ₂ NO (C ₅ H ₃ F ₂ N-H ₂ O)	2,6-difluoropyridine-water complex	Juan Wang ¹	Manuscript in preparation ¹⁸ O, D ₂ O, DOH, HOD isotopes
C ₅ H ₉ F ₄ NS ₂ (C ₃ H ₉ N- C ₂ S ₂ F ₄)	isopropylamine-C ₂ S ₂ F ₄ complex	Yan Jin	Spectra assigned, two conformers
C ₅ H ₁₀ O (C ₅ H ₈ -H ₂ O)	Cyclopentene-H ₂ O	Juan Wang ^{1,2}	MS in preparation, internal rotation of water
C ₅ H ₁₂ OS ₂ (CH ₃ CH ₂ S ₂ CH ₂ CH ₃ - HCHO)	Diethyl Disulfide-H ₂ CO complex	Tao Lu	Spectra assigned, one conformer
C ₅ H ₁₃ NOS ₂ (CH ₃ CH ₂ S ₂ CH ₂ CH ₃ - HCONH ₂)	Diethyl Disulfide-HCONH ₂ complex	Tao Lu	Spectra assigned, one conformer

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₃ FN (2-F-4-CF ₃ C ₆ H ₃)	2-Fluoro-4-methylpyridine	Shuang Gao	Manuscript in preparation, internal rotation of -CH ₃
C ₆ H ₄ S	2-Ethynylthiophene	Yan Jin	Spectra assigned, one conformer
C ₆ H ₄ F ₃ N (2-CF ₃ pyridine)	2-trifluoromethylpyridine	Xiaolong Li	spectra assigned, ¹³ C and ¹⁵ N isotopes
C ₆ H ₅ ClF ₃ N (C ₆ H ₅ -CClF ₃)	pyridine-trifluorochloromethane complex	Qian Gou ^l	Manuscript submitted
C ₆ H ₅ FNO (2-F-4-CF ₃ C ₆ H ₃ -H ₂ O)	2-Fluoro-4-methylpyridine-water complex	Shuang Gao	Spectra assigned, 1 conformer
C ₆ H ₁₄ S ₂ ((CH ₃) ₂ CHS ₂ CH(CH ₃) ₂)	diisopropyl disulfide	Jiaqi Zhang	Spectra assigned, three conformers
C ₇ H ₃ F ₅ (C ₆ F ₅ OCF ₃)	pentafluoroanisole	Xiaolong Li	Spectra assigned, 1 conformer
C ₇ H ₁₀ Si (C ₆ H ₅ SiH ₂ CH ₃)	MethylPhenylSilane	Juncheng Lei	Spectra assigned, one conformer, -CH ₃ internal rotation
C ₇ H ₇ F ₂ N	2,6-Difluorobenzylamine	Shuang Gao	Spectra assigned, one conformer
C ₇ H ₇ F ₂ N	2,4-Difluorobenzylamine	Shuang Gao	Spectra assigned, two conformers, -NH ₂ tunneling
C ₈ H ₅ F ₃ O (C ₆ H ₅ COCF ₃)	2,2,2-trifluoroacetophenone	Juncheng Lei	J. Mol. Spectrosc. 351, 47 (2018).
C ₈ H ₇ F ₃ O ₂ (C ₆ H ₅ COCF ₃ -H ₂ O)	2,2,2-trifluoroacetophenone-water complex	Juncheng Lei	Manuscript in preparation Spectra assigned, 1 conformer
C ₈ H ₈ O	Acetophenone	Juncheng Lei	¹³ C isotopologues, spectra assigned, one conformer, internal rotation of -CH ₃
C ₈ H ₁₀ O (C ₆ H ₅ CHCH ₂ -H ₂ O)	Styrene-water complex	Yang Zheng ⁶	Spectra assigned, one conformer, O ¹⁸ , D ₂ O, DOH, tunneling splitting

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C_4H_4OS (C_4H_3SCHO)	2-Thiophenecarboxaldehyde	Wenqin Li ²	Spectra assigned, two conformers
$C_4H_6O_2S$ ($C_4H_3SCHO-H_2O$)	2-Thiophenecarboxaldehyde-water	Wenqin Li ²	Spectra assigned, two conformers
$C_5H_{10}F_6$ ($CH_2F_2-(CH_3CHF_2)_2$)	$CH_2F_2-(CH_3CHF_2)_2$ trimer	Tao Lu	Spectra assigned, one conformer

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
AgI	silver iodide	L. Bizzocchi ^g , B. M. Giuliano ^g	v = 1 in progress
COSXe (COS...Xe)	carbonyl sulfide ...xenon	S. Herbers D. Wachsmuth D. A. Obenchain P. Kraus	mult. isotopologues assigned, r _e structure
CBr ₂ F ₂	dibromo- difluoromethane	D. A. Obenchain	rot. spectrum, Br nq-hfs
CH ₅ NO ₂ (CH ₂ O ₂ ...H ₃ N)	formic acid ...ammonia	F. Lovas ^a G. T. Fraser ^a R. D. Suenram ^f	conformation, lam spectrum assigned
C ₂ H ₃ NO ₃ (CH ₃ NO...CO ₂)	Formamide ...carbon dioxide	Shuang Gao ^b , D. A. Obenchain, Jungcheng Lei ^b , S. Herbers	N nq-hfs, cd measurements completed accepted <i>Phys. Chem. Chem. Phys.</i>
C ₄ H ₆ F ₄ S ₃ (C ₂ F ₄ S ₂ ...C ₂ H ₆ S)	2,2,4,4-tetrafluoro- 1,3-dithiane ...dimethylsulfide	D. A. Obenchain L. Spada ^g M. Juanes ^e	structure spectrum assigned
C ₂ H ₃ F ₅ O (C ₂ HF ₅ ...H ₂ O)	pentafluoroethane ...water	G. Feng ^b Q. Gou ^b	lam, structure spectrum assigned
C ₂ H ₅ NO	<i>cis</i> N-methyl- formamide	C. Evans ^t , D. McNaughton ^k	N nq-hfs, cd measurements completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₆ Cl ₂ Si	dichloro-dimethylsilane	D. Banser W. Caminati ^g , A. Lesarri ^e , E. J. Cocinero ^o , M. Schnell	lam, Cl nq-hfs analysis in progress
C ₂ H ₆ Cl ₂ Sn	dichloro-dimethylstannane	P. Ottaviani ^g , M. Schnell	lam, Cl nq-hfs spectrum assigned
C ₂ H ₆ ArF ₂ Ge (C ₂ H ₆ F ₂ Ge ···Ar)	difluoro-dimethylgerman ···argon	P. Ottaviani ^g , M. Schnell	lam, ms in preparation
C ₂ H ₆ O ₂ S ₂ (C ₂ H ₆ S···SO ₂)	dimethyl sulfide ···sulfur dioxide	L. Spada ^g D. A. Obenchain S. Herbers, P. Kraus	mult. isotopologues, lam, 33-S nq-hfs <i>Angew. Chem. Int. Ed.</i> 57 , 15822(2018)
C ₃ H ₄ Cl ₂ F ₂ O	methoxyflurane	A. Vega ^e , E. J. Cocinero ^o	conformations, Cl nq-hfs, r _s -structure analysis in progress
C ₃ H ₅ N	propargylamine	L. Bizzocchi ^d V. Lattanzi ^d C. Puzzarini ^g	rot. spec., cd g.s., low vib. states <i>Astron. & Astrophys.</i> 615 , A176(2018).
C ₃ H ₉ ClGe	chloro-trimethylgermane	M. Schnell J. Fritzsche	⁷³ -Ge nq-hfs analysis in progress
C ₄ H ₂ O ₃	succinic anhydride	M. K. Jahn, K. P. R. Nair, D. A. Obenchain, P. Godfrey ^k , D. McNaughton ^k , N. Vogt ^v , J. Demaison ⁿ	rot. spectrum, theor. struct. calc. hfs under study
C ₅ H ₅ F ₃ O ₂ (C ₄ H ₃ F ₃ O ···CH ₂ O)	trifluoroacetone ···formaldehyde	C. Perez ^e A. Lesarri ^e M. K. Jahn, D. Dewald	rot. spectrum, conformations analysis in progress
C ₄ H ₃ F ₃ O ₃	methyl 3,3,3-trifluoropyruvate	D. Siekmann	lam, rot. spec. measurements in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₄ OS	2-thiophene-carboxaldehyde	W. Li ^b	rot. spec., cd, 2 conf. spectra assigned
C ₄ H ₆ O ₂ S (C ₄ H ₄ OS ···H ₂ O)	2-thiophene-carboxaldehyde ...water	W. Li ^b	rot. spec., cd, 2 conf. spectra assigned
C ₄ H ₆ O ₂	vinylacetate	S. Genuit	lam, mult. isotopologues, high K _a analysis in progress
C ₄ H ₆ O ₂	methacrylic acid	S. Herbers P. Kraus	r _e structure accepted <i>J. Chem. Phys.</i>
C ₄ H ₇ NO	acetone-cyanohydrin	K. Aydt, M. J. Travers, M. K. Jahn	N nq-hfs, cd assignment completed
C ₄ H ₁₀ ArS ₂ (C ₄ H ₁₀ S ₂ ···Ar)	diethyl disulfide ···argon	G. Feng ^b	rot. spec., cd spectra assigned
C ₄ H ₁₂ OS ₂ (C ₄ H ₁₀ S ₂ ···H ₂ O)	diethyl disulfide ···water	X. Li ^b	lam, O ¹⁸ , D ₂ O, DOH, HOD spectra assigned
C ₅ HN	pentadiene nitrile	H. Span ^j	measurements completed
C ₅ H ₁₀ O (C ₅ H ₈ ···H ₂ O)	cyclopentene ···water	J. Wang	lam ms in preparation
C ₅ H ₈ O ₂	acetylacetone	W. Caminati ^g , H. G. Kjaergaard ^c	enolic shape, lam deuterated species in progress
C ₅ H ₈ O ₂	methyl methacrylate	S. Herbers D. Wachsmuth D. A. Obenchain	lam, r _s -structure 2 conformers assigned <i>J. Mol. Spectrosc.</i> 343 , 96(2018).
C ₅ H ₈ O ₂	methyl methacrylate	S. Herbers P. Kraus	r _e structure accepted <i>J. Chem. Phys.</i>
C ₅ H ₉ N	3-methylbutyronitrile	N. Wehres ^j , M. Hermanns ^j , O. H. Wilkins ^j , K. Borisov ^j ,	rot. spec., cd, 2 conf. MW, mmW <i>Astron. & Astrophys.</i> 615 , A140(2018)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₅ H ₁₀ O ₃ (C ₅ H ₈ O ₂ ···H ₂ O)	methyl methacrylate ···water	S. Herbers	lam, rot. spec. assignment in progress
C ₁₀ H ₁₆ O ₄ ((C ₅ H ₈ O ₂) ₂)	methyl methacrylate dimer	S. Herbers, D. A. Obenchain, K. G. Lengsfeld, H. Kuper	rot. Spectrum, lam, <i>J. Mol. Spectrosc.</i> 351 , 49(2018).
C ₅ H ₁₆ SiSn	dimethylsilyl- trimethylstannane	J. T. Hougen ^a , M. Schnell	lam assignment in progress
C ₆ H ₃ F ₃ O	3,4,5-trifluoro - phenol	K.P.R. Nair D. A. Obenchain	r _s -structure spectrum assigned
C ₆ H ₃ F ₃ O	3,4,5-trifluoro - phenol	K.P.R. Nair P. Buschman D. A. Obenchain	r _s -structure spectrum assigned
C ₆ H ₄ F ₂ O	2,3-difluoro - phenol	K.P.R. Nair D. Dewald D. Wachsmuth	r _s -structure ms in preparation
C ₆ H ₄ F ₂ O	3,4-difluoro - phenol	K.P.R. Nair	r _s -structure spectrum assigned
C ₆ H ₄ F ₂ O	3,5-difluoro - phenol	D. Dewald	lam analysis completed
C ₆ H ₄ N ₂	2-cyano pyridine	D. Prudenzano, D. Wachsmuth, M. K. Jahn, D. McNaughton ^k	2xN nq-hfs, r _s -structure ms in preparation
C ₆ H ₄ N ₂	3-cyano pyridine	D. Prudenzano, D. Wachsmuth, M. K. Jahn, D. McNaughton ^k	2xN nq-hfs, r _s -structure ms in preparation
C ₆ H ₄ N ₂	4-cyano pyridine	K. P. R. Nair, N. Vogt ^v , J. Demaison ⁿ	2xN nq-hfs, r _s -structure <i>Mol. Phys.</i> 116 , 3530(2018).

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₇ N	4-picoline	S. Herbers, M. K. Jahn, D. Wachsmuth J. Matysik ⁱ V. V. Ilyushin ^p W. Caminati ^g	lam, N nq-hfs, analysis in progress
C ₆ H ₁₁ NO	ε-caprolactam	D. Wachsmuth M. Vallejo ^e	N nq-hfs , pseudo-rot., spectra assigned
C ₆ H ₁₂ O	oxepane	J. Borter, D. Wachsmuth, A. Lesarri ^e	rot. Spectrum, pseudo-rot. spectrum assigned
C ₆ H ₁₃ N	azepane	D. Wachsmuth, M. Vallejo ^e	N nq-hfs, pseudo-rot. spectra assigned
C ₇ H ₅ F ₃	2,3,4-trifluoro- toluene	K. P. R. Nair S. Herbers	lam, Stark effect, r _s -structure ms in preparation
C ₇ H ₆ F ₂	2,3-difluoro- toluene	K. P. R. Nair S. Herbers D. A. Obenchain, A. Lesarri ^e	lam, Stark effect, r _s -structure <i>J. Mol. Spectrosc.</i> 349 , 37(2018).
C ₇ H ₆ F ₂	2,4-difluoro- toluene	K. P. R. Nair S. Herbers D. A. Obenchain, A. Lesarri ^e	lam, Stark effect, r _s -structure <i>J. Mol. Spectrosc.</i> 344 , 21(2018).
C ₇ H ₆ F ₂	3,4-difluoro- toluene	K. P. R. Nair S. Herbers	lam, Stark effect, r _s -structure accepted <i>J. Mol. Spectrosc.</i>
C ₇ H ₇ Cl	ortho-bromo- toluene	K. P. R. Nair S. Herbers, J. Wang, P. Buschmann	lam, Br nq-hfs ms in preparaton
C ₇ H ₇ Cl	ortho-chloro- toluene	K. P. R. Nair S. Herbers, J. Wang, P. Buschmann	lam, Cl nq-hfs ms in preparaton

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₇ H ₇ Cl	<i>meta</i> -chloro-toluene	K. P. R. Nair S. Herbers, A. Lesarri ^e	lam, Cl nq-hfs accepted <i>J. Mol. Spectrosc.</i>
C ₇ H ₇ Cl	<i>para</i> -chloro-toluene	K. P. R. Nair V. V. Ilyushin ^p	lam, Cl nq-hfs ms in preparation
C ₇ H ₇ F	<i>ortho</i> -fluoro-toluene	K. P. R. Nair S. Herbers, J. Wang, P. Buschmann	lam, substituent effects ms in preparaton
C ₇ H ₇ F	<i>meta</i> -fluoro-toluene	K. P. R. Nair S. Herbers	lam, r _s -structure ms in preparaton
C ₇ H ₇ I	<i>ortho</i> -iodo-toluene	K. P. R. Nair S. Herbers, J. Wang, P. Buschmann	lam, I nq-hfs ms in preparaton
C ₇ H ₁₂	cycloheptene	D. Wachsmuth	structure spectrum assigned
C ₇ H ₁₂ O	cycloheptanone	D. Wachsmuth, M. K. Jahn	lam, pseudo-rot. spectrum assigned
C ₈ H ₄ N ₂	1,2-dicyano-benzene	E. Locatelli D. Dewald M. K. Jahn	N nq-hfs, structure, ms in preparation
C ₈ H ₄ N ₂	1,3-dicyano-benzene	D. Dewald M. K. Jahn M. Jüstel F. Lovas ^a	N nq-hfs, structure, ms in preparation
C ₈ H ₈ O	<i>para</i> -tolualdehyde	W. Caminati ^g A. Hight-Walker ^a J. T. Hougen ^a I. Kleiner ^d J. Gauß ^h H. Saal	barrier to internal rotation, ab-initio tors. analysis ms in preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₈ H ₈ O	<i>para</i> -tolualdehyde	W. Caminati ^g A. Hight-Walker ^a J. T. Hougen ^a I. Kleiner ^q H. Saal	lam, torsionally excited states, <i>J. Mol. Spectrosc.</i> 351 , 55(2018).
C ₈ H ₁₂ N	cyanocycloheptane	D. Wachsmuth A. Lesarri ^e	lam, N nq-hfs, conformation ms in preparation
C ₉ H ₆ O ₂	coumarin	H. V. L. Nguyen ^{m,q}	rot. spectrum, r _s -structure ms in preparation
C ₉ H ₇ NO	8-hydroxy-quinoline	D. Wachsmuth, S. Herbers, J. Wang, P. Kraus, D. McNaughton ^k	N nq.hfs, cd r _e structure heavy atom species assigned ms in preparation
C ₉ H ₁₁ N	1,2,3,4-tetrahydro-quinoline	K. Luková ^r , R. Nesvadba ^r , Tereza Uhlikova ^r , Daniel Obenchain, D. Wachsmuth.	rot. spectrum, cd, lowest energy conf. ab-initio conf. analysis <i>Phys. Chem. Chem. Phys.</i> 20 , 14664(2018).
C ₁₁ H ₇ N	1-cyano-naphthalene	M. J. Travers, D. McNaughton ^k M. K. Jahn	N nq-hfs, cd assignment completed
C ₁₁ H ₇ N	2-cyano-naphthalene	M. J. Travers, D. McNaughton ^k M. K. Jahn	N nq-hfs, cd assignment completed
C ₁₁ H ₁₅ NO ₂	butamben	M. Vallejo ^e , W. Caminati ^g , E. J. Cocinero ^o	conformation(s), r _s -structure ms in preparation
C ₁₁ H ₁₅ NO ₂	isobutamben	M. Vallejo ^e , W. Caminati ^g , E. J. Cocinero ^o	conformation(s), r _s -structure ms in preparation
C ₁₃ H ₁₁ NO	benzanilide	S. Herbers, D. Wachsmuth, M. K. Jahn	lam, N nq-hfs <i>J. Mol. Spectrosc.</i> 351 , 8(2018).

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₁₅ H ₉ N	9-cyano-phenanthrene	M. J. Travers, M. K. Jahn D. Wachsmuth, D. McNaughton ^k P. Godfrey ^k	N nq-hfs, cd <i>Mon. Not. R. Astron. Soc.</i> 476 , 5268(2018).
C ₁₅ H ₉ N	9-cyano-anthracene	M. J. Travers, M. K. Jahn D. Wachsmuth, D. McNaughton ^k P. Godfrey ^k	N nq-hfs, cd <i>Mon. Not. R. Astron. Soc.</i> 476 , 5268(2018).
ClFLi ₂	dilithium chloride fluoride	R. J. Mawhorter ^l	structure measurement in progress
ClRb	rubidium chloride	R. J. Mawhorter ^l	isotopologues, fs/hfs Measurement/assignment completed
CsF ₂ Li	lithium caesium difluoride	R. J. Mawhorter ^l	structure measurement in progress
CuI	copper iodide	L. Bizzocchi ^g , B. M. Giuliano ^g	nq-hfs, spin-spin coupling, $\nu = 1$, in progress
FK	potassium flouride	R. J. Mawhorter ^l	isotopologues, fs/hfs Measurement/assignment completed
FPb	lead flouride	R. J. Mawhorter ^l T. J. Sears ^s	isotopologues, fs/hfs, $\nu > 0$ measurement in progress
FRb	rubidium flouride	R. J. Mawhorter ^l	isotopologues, fs/hfs Measurement/assignment completed
FYb	ytterbium flouride	R. J. Mawhorter ^l , T. C. Steimle ^u	isotopologues, fs/hfs, Zeeman effect measurement in progress
F ₂ KLi	lithium potassium difluoride	R. J. Mawhorter ^l	structure assignment completed
F ₂ LiRb	lithium rubidium difluoride	R. J. Mawhorter ^l	structure measurement/assignment in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
HF ₅ OTe	teflin acid	S. Herbers D. A. Obenchain P. Kraus D. Wachsmuth	r _e -structure, <i>J. Chem. Phys.</i> 148 , 194307(2018).
IK	potassium iodide	R. J. Mawhorter ^l	isotopologues, fs/hfs measurement/assignment completed
IRb	rubidium iodide	R. J. Mawhorter ^l	isotopologues, fs/hfs measurement/assignment completed

The Hannover FTMW spectrometer control & analysis software is available at
<http://www.pci.uni-hannover.de/~lgpca/spectroscopy/ftmw> (temporarily down)

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FORMULA	NAME OF COMPOUND	INVESTIGATOR	PRESENT STAGE OF PROGRESS
C ₃ H ₆ O	acetone	with Christen ^a	v ₁₇ MW-DR, JMSp 356 (2019) 1
C ₂ H ₇ P	ethylphosphine		ERHAM analysis for doublets or quartets in vib exc states
C ₄ H ₇ F ₃ Si (C ₄ H ₇ SiF ₃)	Cyclobutyl trifluorosilane	Pate, ^b Durig, Guirgis, ^c Deodhar	FTMW assigned MS in preparation
C ₄ H ₈ Cl ₂ Si (C ₄ H ₇ SiHCl ₂)	Cyclobutyl dichlorosilane	Durig, Brenner	In progress
C ₄ H ₁₀ Si	4-silyl-1-butene	Durig, Panikar, Tubergen ^d	2 conformers assigned
Analysis/Database	Molecular symmetry: Why permutation-inversion (PI) groups don't render the point groups obsolete		JMSp 343 (2018) 34

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_6H_4ArF_2$	Ar-1,3-Difluorobenzene vdW Complex	F. E. Marshall ¹ , R. Dorris ¹² , S. A. Peebles ¹² , R. A. Peebles ¹² , G. S. Grubbs II ¹	<i>J. Phys. Chem. A</i> 122 (2018) 7385.
$C_3H_2BrF_5$	3-Bromo-1,1,1,2,2- Pentafluoropropane	F. E. Marshall ¹ , N. Moon ¹ , T. D. Persinger ¹ , D. J. Gillcrist ¹ , N. E. Shreve ¹ , W. C. Bailey ⁷ , G. S. Grubbs II ¹	<i>Mol. Phys.</i> 117 (2019) 1351.
$C_{10}H_{16}O$	Myrtenol	F. E. Marshall ¹ , G. Sedo ⁸ , G. S. Grubbs II ¹	<i>J. Mol. Spectrosc.</i> 356 (2019) 32.
$AgClD_2$ $AgClDH$ (D_2 -AgCl and HD-AgCl)	Deuterium-Silver Chloride complex	D. A. Obenchain ² , G. S. Grubbs II ¹ , D. S. Frank, H. M. Pickett ² , S. E. Novick ²	Manuscript in Prep.
$C_{11}H_{18}O$	Nopol	F. E. Marshall ¹ , G. Sedo ⁸ , G. S. Grubbs II ¹	Manuscript in Prep.
C_3ClF_6O	Chloroperfluoroacetone	W.C. Bailey ⁷ , S.A. Cooke ⁴ , G.S. Grubbs II ¹	Manuscript in Prep. with $C_3Cl_2F_4O$
$C_3Cl_2F_4O$	1,3-dichloro-1,1,3,3- tetrafluoroacetone	W.C. Bailey ⁷ , S.A. Cooke ⁴ , G.S. Grubbs II ¹	Manuscript in Prep. with C_3ClF_6O

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_2ClF_3O$	1-chloro-3,3,3-trifluoroacetone	S. A. Cooke ⁴ and G. S. Grubbs II ¹	Manuscript in Prep.
BaS	Barium Monosulfide	G. S. Grubbs II ¹ , C. T. Dewberry ⁵ , K. C. Etchison ⁶ , S. A. Cooke ⁴	Manuscript in Prep.
$C_4H_6F_2Si$	1,1-Difluorosilacyclopent-2-ene	F. Marshall ¹ , G. Jones ¹⁰ , T. Carrigan-Broda ¹⁰ , G. Guirgis ¹⁰ , J. Laane ¹⁸ , G. S. Grubbs II ¹	Submitted: <i>J. Phys Chem A</i>
$C_4H_6F_2Si$	1,1-Difluorosilacyclopent-3-ene	F. Marshall ¹ , A. J. Duerden ¹ , G. Jones ¹⁰ , T. Carrigan-Broda ¹⁰ , G. Guirgis ¹⁰ , G.S. Grubbs II ¹	Manuscript in Prep.
$C_4H_8F_2Si$	1,1-Difluorosilacyclopentane	F. E. Marshall ¹ , D. J. Gillcrist ¹ , G. Jones ¹⁰ , T. Carrigan-Broda ¹⁰ , G. Guirgis ¹⁰ , G. S. Grubbs II ¹	Manuscript in Prep.
C_4H_8Si	Silacyclopent-3-ene	F. Marshall ¹ , N. Moon ¹ , G. Jones ¹⁰ , T. Carrigan-Broda ¹⁰ , G. Guirgis ¹⁰ , G.S. Grubbs II ¹	Manuscript in Prep.
$C_5H_{10}ClFSi$	1-Fluoro-1-chloromethylsilacyclopentane	F. Marshall ¹ , G. Jones ¹⁰ , T. Carrigan-Broda ¹⁰ , G. Guirgis ¹⁰ , G. S. Grubbs II ¹	Experiments Completed; Assignments in Progress
C_2HBrF_4	2-Bromo-1,1,1,2-tetrafluoroethane	F. E. Marshall ¹ , J. Isert ¹ , G. S. Grubbs II ¹	Manuscript in Prep.
$C_4H_6F_3I$	3-iodo-1,1,1-trifluorobutane	F. E. Marshall ¹ , J. Isert ¹ , G. S. Grubbs II ¹	Assignment of Parent Completed; ¹³ C's in progress
$ClCuH_2$ (H_2-CuCl)	Hydrogen-Copper Chloride complex	D. Obenchain ² , G. S. Grubbs II ¹ , H. Pickett ² , S. Novick ²	Experiments Completed; Assignments in Progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CF ₂ I ₂	Difluorodiiodomethane	G. S. Grubbs II ¹ and S. A. Cooke ⁴	Experiments Completed; Assignments in Progress
C ₃ H ₅ ClO	Chloroacetone	F. E. Marshall ¹ , S. A. Cooke ⁴ , G. S. Grubbs II ¹	Experiments Completed; Assignments in Progress
C ₂ H ₁₂ Si ₃	Trisilylpentane	F. E. Marshall ¹ , W. R. N. Tonks ¹⁰ , D. J. Gillcrist ¹ , C. J. Wurrey ⁹ , G. Guirgis ¹⁰ , I. Kleiner ¹⁹ , J. Atef ¹⁹ , G. S. Grubbs II ¹	Experiments Completed; Initial Fits Made of Multiple Conformers; Int. Rot. Parameters being Determined
C ₃ H ₇ F ₅ O ₅ (C ₃ HF ₅ O ₂ -(H ₂ O) ₃)	Perfluoropropionic Acid Trihydrate Complex	G. S. Grubbs II ¹ , D. A. Obenchain ² , S. A. Cooke ⁴ , S. E. Novick ² , A. Serrato III ³ , W. Lin ³	Experiments Completed; Assignments in Progress
H ₂ O ₃ (H ₂ O-O ₂)	Water-Oxygen vdW complex	A. J. Duerden ¹ , F. E. Marshall ¹ , N. Moon ¹ , T. D. Persinger ¹ , G. S. Grubbs II ¹	Experiments Completed; Assignments in Progress
C ₁₄ H ₂₀ O	Verbenone-3-butyn-2-ol vdW Complex (chiral tag)	L. Evangelisti ¹⁴ , K. Mayer ¹³ , M. Holdren ¹³ , T. Smart ¹³ , C. West ¹³ , B. Pate ¹³ , G. Sedo ⁸ , F. Marshall ¹ , G. S. Grubbs II ¹	Assignments in Progress
ClPb	Lead Monochloride	G. S. Grubbs II ¹ , S. Norman ¹ , R. Dawes ¹ , B. E. Long ² , C. T. Dewberry ⁵ , S. A. Cooke ⁴	Experiments Completed; Assignments in Progress
CO ₃ (CO-O ₂)	Carbon Monoxide-Oxygen vdW complex	F. E. Marshall ¹ , D. J. Gillcrist ¹ , N. Moon ¹ , T. D. Persinger ¹ , G. S. Grubbs II ¹	Experiments in Progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
ClHO ₂ (HCl-O ₂)	Hydrogen Chloride-Oxygen vdW complex	A. J. Duerden ¹ , F. E. Marshall ¹ , D. J. Gillcrist ¹ , N. Moon ¹ , T. D. Persinger ¹ , G. S. Grubbs II ¹	Experiments Completed; Assignments in Progress
CO ₃ S (OCS-O ₂)	Carbonyl Sulfide-Oxygen vdW Complex	A. J. Duerden ¹ , F. E. Marshall ¹ , N. Moon ¹ , S. Blanco ²⁰ , C. Whitham ²¹ , H. Qian ²¹ , S. Low ²¹ , B. Howard ²¹ , G. S. Grubbs II ¹	Experiments Completed; Assignments in Progress
EXPERIMENTAL	Multiple Antennae Design CP-FTMW (MAD-CP-FTMW)	F. E. Marshall ¹ , A. J. Duerden ¹ , N. Moon ¹ , J. Isert ¹ , G. S. Grubbs II ¹	Submitted: <i>Rev. Sci. Instrum.</i>
EXPERIMENTAL	Low-Cost Balle-Flygare FTMW Experiment	A. J. Duerden ¹ , N. Moon ¹ , F. E. Marshall ¹ , G. S. Grubbs II ¹	Manuscript in Prep. with Teaching Laboratory
ANALYSIS/DATABASE	Rotational Spectroscopy Teaching Laboratory	N. Moon ¹ , A. J. Duerden ¹ , F. E. Marshall ¹ , G. S. Grubbs II ¹	Manuscript in Prep. with Low-Cost Balle-Flygare FTMW

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₃ (HDCCH)	Vinyl	M. Hayashi H. Matsubayashi	Pure rotational transitions for the cis-tautomer assigned and analyzed. Manuscript in preparation.
C ₂ D ₃ (D2CCD)	Vinyl	M. Ohtsuki H. Matsubayashi	Proton tunneling transitions assigned and analyzed. Manuscript in preparation.
CCoO (CoCO)	Cobalt carbonyl	T. Hikida M. Hayashi	Rotational spectrum in the $\Omega = 3/2$ and $5/2$ spin states and vibrationally excited states assigned and analyzed. Manuscript in preparation.
FeNO	Iron nitrosyl	M. Nakashima S. Ikeda	Rotational spectrum in the ground and vibrationally excited states assigned.
C ₇ H ₆ O ₂ (C ₇ H ₅ O ₂ D)	Tropolone	H. Matsumoto	Pure rotational transitions. Manuscript in preparation.
C ₇ H ₆ O ₂ (C ₇ H ₅ O ₂ D)	Tropolone	K. Tanaka Y. Endo	FTMW spectra of tunneling rotation transitions. Manuscript in preparation.
C ₇ H ₆ O ₂ (¹³ CC ₆ H ₆ O ₂)	Tropolone	K. Tanaka Y. Endo	Pure rotational and tunneling rotation transitions of ¹³ C isotopic substituted species. Manuscript in preparation.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₃ H ₄ O ₂	Malonaldehyde	T. Baba K. Tanaka	Proton tunneling spectrum. Collaboration with Dr. K.M.T. Yamada (NIRE). Millimeterwave spectrum of internal rotation hot band and intermolecular stretching band. Munuscript in preparation.
CHHeN (He-HCN)	Helium-hydrogen cyanide complex	K. Harada K. Tanaka	Millimeterwave spectrum of internal rotation fundamental and hot bands.
CHHeN (He-DCN)	Helium-hydrogen cyanide complex	K. Harada M. Takagi M. Takamori	Millimeterwave spectrum of internal rotation fundamental and hot bands.
CHNNe (Ne-HCN)	Neon-hydrogen cyanide complex	K. Harada A. Okumura K. Hagi	Millimeterwave spectrum of internal rotation bands. Munuscript in preparation.
CHNNe (Ne-DCN)	Neon-hydrogen cyanide complex	M. Takagi N. Oyamada	Millimeterwave spectrum of internal rotation bands.
CHArN (Ar-HCN)	Argon-hydrogen cyanide complex	S. Matsushita	Millimeterwave spectrum of the $j=3-2$ internal rotation band.
CHArN (Ar-DCN)	Argon-hydrogen cyanide complex	R. Watanabe	Millimeterwave spectrum of the $j=2-1$ internal rotation band.
CH ₃ N (H ₂ -HCN)	Hydrogen-hydrogen cyanide complex	K. Hagi R. Yamanaka M. Ishiguro K. Harada K. Tanaka	Millimeterwave absorption spectrum of internal rotation band observed and assigned.
CH ₃ N (H ₂ -DCN)	Hydrogen-hydrogen cyanide complex	M. Ishiguro K. Harada K. Tanaka T. Tanaka M. Nakajima Y. Sumiyoshi Y. Endo	FTMW and MMW spectra have been observed and analyzed. Manuscript in preparation.
ClH ₃ (H ₂ -HCl)	Hydrogen-hydrogen chloride complex	M. Ishiguro	Pure rotational spectrum assigned and analyzed.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
ClH ₃ (H ₂ -DCl)	Hydrogen-hydrogen chloride complex	K. Nagata	Pure rotational spectrum observed and analyzed.
FH ₃ (H ₂ -HF) (H ₂ -DF)	Hydrogen-hydrogen fluoride complex	T. Moriyama Y. Iwasaki	Pure rotational spectrum observed.
CHFO ₂ (OCO-HF) (OCO-DF)	Carbon dioxide-hydrogen fluoride complex	K. Harada M. Ishiguro C. Whitham	Millimeterwave spectrum of vdw bend band.
H ₄ O (H ₂ -H ₂ O) (H ₂ -D ₂ O)	Hydrogen-water complex	K. Harada C. Whitham Y. Iwasaki T. Giesen K. Tanaka	Pure rotational millimeterwave spectrum observed. Manuscript in preparation.
C ₂ H ₂ N ₂ (HCN-DCN) (DCN-HCN) (DCN-DCN)	Hydrogen cyanide dimer	K. Harada M. Shirasaka K. Tanaka	Millimeterwave spectrum of high- <i>J</i> rotational lines. Manuscript in preparation.
C ₂ H ₂ N (CH ₂ CN)	Cyanomethyl radical	M. J. Tsuchiya	Spectrum in excited vibrational states observed.
Cl ₂ Sn (SnCl ₂)	Tin dichloride	K. Uemura	Spectrum assigned.
FGe ⁺ (GeF ⁺)	Germanium fluoride ion	K. Tanaka	In progress
C ₃ H ₆	Cyclopropane	K. Tanaka	Centrifugal distortion induced transitions.
C ₃ H ₄	Allene	K. Tanaka	Vibrationally induced transitions. Manuscript in preparation.
F ₃ OP (POF ₃)	Phosphoryl fluoride	K. Someya	LMDR in excited states in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
F ₃ HSi (HSiF ₃) (DSiF ₃)	Trifluorosilane	K. Harada	LMDR Manuscript in preparation.
CH ₃ F (CH ₃ F) (CD ₃ F)	Methyl fluoride	K. Harada	LMDR Manuscript in preparation.
CH ₃ I	Methyl iodide	K. Harada	LMDR in progress.
C ₂ HF (HCCF)	Fluoroacetylene	Y. Nakahara	LMDR in progress.
C ₂ H ₃ N (CH ₃ CN)	Methyl cyanide	T. Oyama	LMDR in progress.
C ₂ H ₃ N (CH ₃ NC)	Methyl isocyanide	T. Oyama	LMDR Manuscript in preparation.
C ₃ HN (DCCCN)	Cyanoacetylene	K. Tanaka	LMDR in progress.
CFN (FCN)	Cyanogen fluoride	S. Matsuba	LMDR in progress.
ClF ₅ S (SClF ₅)	Sulfur chloride pentafluoride	K. Harada	LMDR in progress.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₁₀ S	7-Thiabicyclo [2.2.1]heptane	K. Irie	Work in progress.
HNO	Nitroxyl	K. Takagi ^b S. Saito ^c	Manuscript in preparation.
ClOS[ClSO]	ClSO radical	S. Saito ^c	Work almost completed.
CH ₃ O ₂ [CH ₃ OO]	Methyl peroxide	K. Katoh ^d Y. Endo ^d E. Hirota	Manuscript in preparation.
C ₄ H ₆ D ₂	Cyclobutane-1,2-d ₂	E. Hirota	<i>cis, trans</i> , work completed.
C ₄ H ₄ D ₄	Cyclobutane-1,1,3,3,-d ₄	E. Hirota	Work completed.
KO	Potassium monoxide	C. Yamada	² Π, ² Σ ⁺ , work almost completed.
BH ₄ N	Aminoborane	W. Lewis-Bevan	Work almost completed.
BH ₄ Li	Lithium tetrahydroborate	Y. Kawashima ^a	Excited vibrational states, work in progress.
BH ₄ K	Potassium tetrahydroborate	Y. Kawashima ^a	Excited vibrational states, work almost completed.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₆ N ₂ O [N ₂ -(CH ₃) ₂ O]	Dinitrogen-dimethyl ether	Y. Kawashima ^a E. Hirota	Spectra assigned for N ₂ , N ¹⁵ N, ¹⁵ N ₂ species.
C ₃ H ₆ N ₂ O ₂ prepared. [NH ₂ COCH ₂ CONH ₂]	Malonamide	T. Usami ^a Y. Kawashima ^a R. D. Suenram ^e E. Hirota	Manuscript
C ₃ H ₆ O [CH ₃ CH(O)CH ₂]	Propylene oxide	E. Hirota Y. Kawashima ^a	Work completed.
C ₃ H ₆ O ₂ S [CO ₂ -(CH ₃) ₂ S]	Carbon dioxide-dimethyl-sulfide	S. Iwano ^a Y. Kawashima ^a E. Hirota	Work in progress, two states assigned.
C ₃ H ₇ NO [HCONHCH ₂ CH ₃]	<i>N</i> -Ethylformamide	K. Ohba ^a T. Usami ^a Y. Kawashima ^a E. Hirota	Second conformer assigned.
C ₃ H ₈ OS [OHCH ₂ CH ₂ CH ₂ SH]	3-Mercapto-1- propanol	Y. Tanaka ^a Y. Kawashima ^a E. Hirota	Five rotamers assigned.
C ₄ H ₆ O ₂ [CO-CH ₃ CH(O)CH ₂]	Carbon monoxide -propylene oxide	H. Mizuno ^a Y. Kawashima ^a E. Hirota	<i>Anti</i> form: normal, ¹³ C, C ¹⁸ O species, assigned.
C ₄ H ₆ O ₃ [CH ₃ CH(CO ₃)CH ₂]	Propylene carbonate	T. Kinjo ^a Y. Kawashima ^a E. Hirota	Normal, ¹³ C (4 species), ¹⁸ O (3 species) assigned.
C ₄ H ₇ NO ₂ [(CH ₃ CO) ₂ NH]	Diacetamide	Y. Kawashima ^a R. D. Suenram ^e E. Hirota	<i>A</i> state and <i>E</i> state assigned.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₈ N ₂ O ₂ [CH ₃ CONHCH ₂ CONH ₂]	<i>N</i> _α -Acetylglycinamide	Y. Kawashima ^a R. J. Lavrich ^e R. D. Suenram ^e E. Hirota	<i>A</i> state assigned, <i>E</i> state assignment in progress.
C ₄ H ₉ NO prepared. [CH ₃ CONHCH ₂ CH ₃]	<i>N</i> -Ethylacetamide	Y. Kawashima ^a T. Usami ^a K. Ohba ^a R. D. Suenram ^e E. Hirota	Manuscript
C ₄ H ₁₀ O [CH ₃ CH ₂ CH ₂ CH ₂ OH]	<i>n</i> -Butanol	T. Uzuyama ^a Y. Tanaka ^a Y. Kawashima ^a E. Hirota	Seven rotamers assigned.
C ₄ H ₁₀ O [CH(CH ₃) ₂ CH ₂ OH]	Isobutanol	T. Uzuyama ^a Y. Kawashima ^a E. Hirota	Four rotamers assigned.
C ₄ H ₁₀ S [CH ₃ CH ₂ CH ₂ CH ₂ SH]	<i>n</i> -Butanethiol	Y. Tanaka ^a Y. Kawashima ^a E. Hirota	Seven rotamers, one for SD assigned.
C ₄ H ₁₀ S [CH(CH ₃) ₂ CH ₂ SH]	Isobutanethiol	Y. Tanaka ^a Y. Kawashima ^a E. Hirota	Three rotamers, ³⁴ S, ¹³ C species assigned.
C ₅ H ₁₀ O [<u>CH₂CH₂CH₂CH₂CHOH</u>]	Cyclopentanol	Y. Kawashima ^a E. Hirota B. Carroll ^f G. Blake ^f	Work in progress
C ₅ H ₁₂ O [CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ OH]	<i>n</i> -pentanol	Y. Komamine ^a Y. Kawashima ^a E. Hirota	Six isomers assigned.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₅ H ₁₂ O [H ₃ CCH ₂ CH(CH ₃)CH ₂ OH]	2-Methyl-1-butanol	Y. Kawashima ^a N. Koshimae ^a Y. Tanimoto ^a E. Hirota	Three conformers assigned.
C ₅ H ₁₂ S [(CH ₃) ₃ CSCH ₃]	<i>Tert</i> -butyl methyl sulfide	R. Watanabe ^a Y. Kawashima ^a E. Hirota	Normal, ³⁴ S, ¹³ C species assigned.
C ₆ H ₁₀ assigned. [CH=CHCH ₂ CH ₂ CH ₂ CH ₂]	Cyclohexene	Y. Kawashima ^a E. Hirota	Isotopomer
C ₆ H ₁₀ O [CH ₃ CH ₂ CH ₂ CH=CHCHO]	<i>Trans</i> -2-hexenal	R. Yokoyama ^a Y. Kawashima ^a E. Hirota	Four conformers assigned
C ₆ H ₁₄ O [CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ OH]	<i>n</i> -Hexanol	Y. Hosoya ^a Y. Kawashima ^a E. Hirota	Three conformers assigned
C ₈ H ₁₂ [CH=CHCH ₂ CH(CH=CH ₂)CH ₂ CH ₂]	4-Vinyl-1-cyclohexene	Y. Nakanishi ^a Y. Kawashima ^a R. J. Lavrich ^e R. D. Suenram ^e E. Hirota	Two conformers assigned.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₇ H ₇ Cl (CH ₃ C ₆ H ₄ Cl)	p-chlorotoluene	Ilyushin V. ^{a,b}	FTMW spectrum of the ³⁵ Cl and ³⁷ Cl isotopologues, analysis in progress
C ₃ H ₄ O ₃ (CH ₃ COCOOH)	pyruvic acid	Ilyushin V. ^{a,c} Alekseev E.	Measurements in the 49-149 GHz range; gs + v _t =1 state assigned, v ₂₄ in progress.
C ₂ H ₅ NO (CH ₃ CONH ₂)	acetamide	Ilyushin V. ^d	Measurements in the 49-660 GHz range; analysis of v _t =0,1,2 up to J=60 in progress.
C ₃ H ₆ O ₂ (C ₂ H ₅ COOH)	propionic acid	Ilyushin V. ^e	Microwave spectrum in the 150 – 540 GHz range, v _t =0 spectrum assigned, analysis in progress
CH ₃ D ₂ N (CH ₃ ND ₂)	deuterated methylamine	Ilyushin V. ^e Alekseev E.	Measurements in the 50-950 GHz range, spectrum assigned, analysis in progress.
C ₃ H ₆ O ₂	2-furan-methanol	Alekseev E. ^e Dyubko S.	Microwave spectrum in 5 – 210 GHz frequency range, analysis in progress
C ₃ H ₄ O ₃	2-furan-carboxylic acid	Alekseev E. ^e	Microwave spectra in the 5 - 240 GHz, manuscript in preparation
C ₃ H ₇ NO (CH ₃ CH ₂ CONH ₂)	propionamide	Ilyushin V. ^e Alekseev E.	MM+SMM spectra, internal rotation, analysis in progress
C ₂ H ₄ O ₂ (HCOOCH ₃)	methylformate	Ilyushin V. ^e	gs and first excited torsional state, 49-950 GHz, v _t =2 analysis in progress
C ₃ H ₆ O ((CH ₃) ₂ CO)	acetone	Ilyushin V. ^e Alekseev E.	Measurements in the 49-950 GHz, v _t =0,1,2 assigned up to J=90, manuscript in preparation; v _t =3,4 analysis in progress.
C ₄ H ₄ O CH ₃ CCCHO	2-butylnal	Ilyushin V. ^e	Measurements in the 3-215 GHz range, analysis in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₆ S (CH ₃) ₂ S)	dimethylsulfide	Ilyushin V. ^{c,e} Aleksseev E.A.	Measurements in the 49 – 660 GHz range, analysis of the $v_t=0,1,2$ microwave data up to $J=60$, manuscript in preparation
CH ₄ O (CH ₃ OH)	methanol	Aleksseev E. ^{g,h,i}	anomalous hyperfine splittings of high J transitions in $v_t=1$ published JMS 357, 11-23 (2019); $v_t=2$ analysis in progress.
C ₂ H ₄ O (CH ₃ CHO)	acetaldehyde	Ilyushin V. ^{e,c,g}	Analysis of the $v_{10}=1$ and $v_t=3,4$ torsional states in the 49 – 960 GHz range is in progress.
C ₂ H ₄ S (CH ₃ CHS)	thio-acetaldehyde	Ilyushin V. ^e	Analysis of the new measurements in the 150 – 660 GHz range, manuscript in preparation
CH ₅ As (CH ₃ AsH ₂)	methylarsine	Ilyushin V. ^e	Analysis of the mm and submm spectra up to 650 GHz, manuscript in preparation
CH ₄ S (CH ₃ SH)	methyl mercaptan	Ilyushin V. ^d	Measurements in the 49 – 500 GHz range, analysis of the $v_t=0,1,2$ microwave data up to $J=60$, manuscript in preparation; $v_t=3,4$ and CS stretch MW spectra analysis in progress
CH ₄ S (CH ₃ ³⁴ S)	³⁴ S methyl mercaptan	Ilyushin V. ^d	Measurements in the 49 – 500 GHz range, analysis of the $v_t=0,1,2$ states, manuscript in preparation
CH ₄ S (¹³ CH ₃ SH)	¹³ C methyl mercaptan	Ilyushin V. ^d	Measurements in the 49 – 500 GHz range, analysis of the $v_t=0,1,2$ in progress.
CH ₄ S (CH ₃ SD)	SD methyl mercaptan	Ilyushin V. ^d	New measurements in the 150 – 510 GHz range, analysis of the $v_t=0,1,2$ states, published A&A 621, A114 (2019).
C ₂ H ₄ OS (HSCOCH ₃)	O-methyl thioformate	Ilyushin V. ^e	gs and first excited torsional state, 150-650 GHz, analysis in progress.
C ₂ H ₅ N (CH ₃ CHNH)	ethanimine	Ilyushin V. ^e	Measurements in the 75 – 650 GHz range, analysis of E and Z conformers in the $v_t=0,1,2$ torsional states in progress

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
H_2N_2O (oH_2-N_2O ; pH_2-N_2O ; pD_2-N_2O ; $^{15}N, ^{15}N_2$)	dihydrogen - nitrous oxide	J. N. Landry	Manuscript in preparation. ¹
$H_2N_N_2O$, $N=2-12$ (oH_2 ; pH_2 ; ^{15}N ; $^{15}N_2$)	(dihydrogen) _N - nitrous oxide	J. N. Landry	Manuscript in preparation.
H_3NNe (Ne - NH_3)	neon - ammonia (inversion transitions)	J. M. Michaud L. E. Downie P. Raston	Spectra collected; assignment in progress.
CFHeN (He-FCN)	helium – fluorine cyanide	M. Morissey C. Knapp	PES calculated; spectra collected.
$C_2H_6O_6$ ($C_2H_2O_4-(H_2O)_2$)	oxalic acid - (water) ₂	E. Schnitzler	Manuscript near completion.
$C_2H_6F_3NO$ ($C_2H_3F_3O-NH_3$)	trifluoroethanol-ammonia	J. Thomas Y. Yang	Manuscript near completion. ²
$C_2H_{10}O_5$ ($C_2H_4O_2-(H_2O)_3$)	acetic acid – water ₃	E. Schnitzler N. Seifert	ab initio calculations completed assignment in progress.
$C_3H_8O_2$ ($C_3H_6O-H_2O$)	acetone - water	J. Gao J. Thomas	Manuscript near completion. ²
$C_3H_8O_3$ ($C_3H_6O_2-H_2O$)	hydroxyacetone - water	E. Schnitzler N. Seifert J. Thomas	ab initio calculations completed assignment in progress.
$C_4H_4N_2O$	4-hydroxypyrimidine	J. Gao	2 tautomers identified
$C_4H_4O_2$	2-furanol	X. Dong N. Seifert	ab initio calculations completed assignment in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_4H_6N_2O_2$ ($C_4H_4N_2O-H_2O$)	4-hydroxypyrimidine - water	J. Gao	ab initio calculations completed assignment in progress.
$C_4H_6O_3$	2-furanol - water	X. Dong N. Seifert	ab initio calculations completed assignment in progress.
C_4H_7NO ($C_4H_5N-H_2O$)	pyrrole - water	B. Wu J. Thomas	^{13}C isotopologues; spectra assigned. ²
$C_4H_9NO_2$ ($C_4H_5N-(H_2O)_2$)	pyrrole - (water) ₂	B. Wu J. Thomas	ab initio calculations; assignment in progress. ²
$C_5H_5He_N N$ ($N=1-19$) ($C_5H_5N-He_N$)	pyridine - He_N ($N=1-19$)	A. Hazrah N. Seifert	Spectra assigned; manuscript in preparation. ³
$C_5H_5N_3$ ($C_5H_5N-N_2$)	pyridine - nitrogen	C. Tanjaroon	Manuscript in preparation.
C_5H_7N ($C_5H_5N-H_2$)	pyridine - hydrogen	C. Tanjaroon	Manuscript in preparation.
$C_5H_{10}O_3$ ($C_5H_8O_2-H_2O$)	acetylacetone - water	J. Gao	ab initio calculations completed partial assignment.
$C_5H_{10}O_4$ ($C_5H_8O_3-H_2O$)	tetrahydro-2-furoic acid - water	F. Xie N. Seifert	Spectra assigned; manuscript in preparation. ²
$C_6H_{10}O_2$ ($C_6H_{10}O-H_2O$)	cyclohexanone - H_2O	J. Gao N. Seifert	Manuscript submitted.
$C_6H_{10}O_3$ ($C_6H_8O_2-H_2O$)	1,3-cyclohexanedione - H_2O	J. Gao	ab initio calculations completed assignment in progress.
$C_6H_{12}O_4$ ($(C_3H_6O_2)_2$)	(hydroxyacetone) ₂	E. Schnitzler N. Seifert J. Thomas	ab initio calculations completed assignment in progress.
$C_6H_{12}O_6$ ($(C_3H_6O_3)_2$)	glycerol dimer (propane-1,2,3-triol) ₂	F. Xie N. Seifert	Several dimers assigned. ²
$C_7H_5He_N N$ ($N=1-8$) ($C_7H_5N-He_N$)	benzonitrile - He_N ($N=1-8$)	A. Hazrah N. Seifert	Spectra assigned; manuscript in preparation. ³
$C_8H_{10}O_3$ ($C_8H_8O_2-H_2O$)	<i>m</i> -toluic acid - water	E. Schnitzler N. Seifert M. Al-Jabiri	ab initio calculations completed assignment in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_8H_{11}NO_3$ ($C_8H_8O_3-NH_3$)	methyl salicylate - ammonia	J. Thomas J. Kwak	Ab initio calculations complete assignment in progress. ²
$C_{10}H_8O$	1-, 2-naphtol	A. Hazrah N. Seifert	manuscript near completion.
$C_{10}H_8NeO$ ($C_{10}H_8O-Ne$)	1-, 2-naphtol - Ne	A. Hazrah N. Seifert	Ab initio calculations complete assignment completed.
$C_{10}H_{10}O_2$ ($C_{10}H_8O-H_2O$)	1-, 2-naphtol - water	A. Hazrah N. Seifert	Ab initio calculations complete assignment completed.
$C_{10}H_{18}O$ ($C_{10}H_{16}-H_2O$)	α -pinene - water	A. Hazrah	Ab initio calculations complete assignment in progress.
$C_{10}H_{16}O$	perillyl alcohol	F. Xie N. Seifert M. Heger J. Thomas	Conformers assigned; manuscript near completion. ²
$C_{10}H_{16}O_6$ ($C_5H_8O_3$) ₂	(tetrahydro-2-furoic acid) ₂	F. Xie N. Seifert	Dimer assigned; manuscript in preparation. ²
$C_{10}H_{18}O_2$ ($C_{10}H_{16}O-H_2O$)	perillyl alcohol - water	F. Xie N. Seifert	Assignment in progress. ²
$C_{10}H_{18}O_4$ ($C_{10}H_{16}O_3-H_2O$)	pinonic acid - water	A. Hazrah E. Schnitzler	Assignment in progress.
$C_{12}H_{14}O_4$	diethyl phthalate	H. T. Tran N. Seifert	Spectrum assigned.

¹ In collaboration with Professor Yasuki Endo, National Chiao Tung University, Taiwan.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ F ₆ O ₂ (^{12/13} CF ₃ OOCF ₃)	Bis(trifluoromethyl) peroxide ¹³ C isotopologue	Kang; Novick Kang; Novick	Presentation in ISMS Searching for ¹⁸ O-iso
C ₂ F ₂ N	1,1-difluorocyanomethyl radical	Kang; Novick	Spectrum assigned Presentation in ISMS
C ₃ F ₆ O	Hexafluoropropylene	Kang; Shipman; Pate	Spectrum assigned Presentation in ISMS
C ₄ DNO ₂	Deuterated T-shaped carbon dioxide cyanoacetylene complex	Kang; Novick; Kukolich	Transitions observed working on hf structures
C ₃ HN ₃	Linear nitrogen-cyanoacetylene complex	Kang; Novick	Spectrum assigned working on hf structures
C ₆ HDN ₂	HCCCN---DCCCN complex	Kang; Novick; Kukolich	Spectrum assigned working on hf structures
C ₆ HDN ₂	DCCCN---HCCCN complex	Kang; Novick; Kukolich	Spectrum assigned working on hf structures
C ₆ D ₂ N ₂	DCCCN dimer complex	Kang; Novick; Kukolich	Spectrum assigned working on hf structures
C ₃ F ₆ O	Perfluoromethylvinylether	Kang; Brown; Pate	Spectrum assigned
C ₇ H ₃ F ₅ O	2,3,4,5,6-perfluoroansiol	Kang; Pate	Spectrum assigned
C ₃ H ₁₀ Si	Trimethylsilane	Kang; Novick	Spectrum assigned Manuscript in preparation
C ₅ H ₁₀ SiH	Trimethylsilylacetylene	Kang; Novick	Spectrum assigned Presentation in ISMS Manuscript in preparation
C ₇ H ₁₀ Si	Trimethylsilyldiacetylene	Kang; Novick	Spectrum assigned Presentation in ISMS Manuscript in preparation
C ₆ H ₉ NSi	Trimethylsilylacetylene cyanide	Kang; Novick	Spectrum assigned Presentation in ISMS Manuscript in preparation
C ₃ H ₃ NSi	Silylacetylene cyanide	Kang; Novick	Spectrum observed Work in progress

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
BH ₄ Li [LiBH ₄]	Lithium tetrahydroborate	Y. Kawashima E. Hirota ^a	Excited vibrational states, work in progress.
BH ₄ K [KBH ₄]	Potassium tetrahydroborate	Y. Kawashima E. Hirota ^a	Excited vibrational states, work almost completed.
CH ₆ O [CD ₄ -- H ₂ O, HDO, D ₂ O]	Methane-water	Y. Kawashima L.H.Coudert ^c	Manuscript prepared
C ₂ H ₄ N ₂ S [N ₂ -(CH ₂) ₂ S]	Dinitrogen-ethylene sulfide	S. Iwano Y. Kawashima E. Hirota ^a	<i>J. Phys. Chem. A</i> 122 (2018) 9454
C ₂ H ₆ N ₂ O [N ₂ -(CH ₃) ₂ O]	Dinitrogen-dimethyl ether	Y. Kawashima E. Hirota ^a	Spectra assigned for N ₂ , N ¹⁵ N, ¹⁵ N ₂ species.
C ₂ H ₆ N ₂ S [N ₂ -(CH ₃) ₂ S]	Dinitrogen-dimethyl sulfide	S. Iwano Y. Kawashima E. Hirota ^a	<i>J. Phys. Chem. A</i> 122 (2018) 9454
C ₃ H ₅ NO [CH ₂ =CHCONH ₂]	Acrylamide	T. Usami Y. Kawashima	Isotopomers assigned
C ₃ H ₆ N ₂ O ₂ [NH ₂ COCH ₂ CONH ₂]	Malonamide	T. Usami E. Hirota ^a R. D. Suenram ^b	Manuscript prepared.
C ₃ H ₆ O [CH ₃ CH(O)CH ₂]	Propylene oxide	E. Hirota ^a Y. Kawashima	Work completed.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₃ H ₆ O ₂ S [CO ₂ -(CH ₃) ₂ S]	Carbon dioxide-dimethyl-sulfide	Y. Kawashima S. Iwano E. Hirota ^a	Work in progress, two states assigned.
C ₃ H ₇ NO [HCONHCH ₂ CH ₃]	<i>N</i> -Ethylformamide	K. Ohba T. Usami Y. Kawashima E. Hirota ^a	Second conformer assigned.
C ₃ H ₈ OS [OHCH ₂ CH ₂ CH ₂ SH]	3-Mercapto-1- propanol	Y. Tanaka Y. Kawashima E. Hirota ^a	Five rotamers assigned.
C ₄ H ₆ O ₂ [CO-CH ₃ CH(O)CH ₂]	Carbon monoxide -propylene oxide	Y. Kawashima H. Mizuno E. Hirota ^a	<i>Anti</i> form: normal, ¹³ CO, C ¹⁸ O species, assigned.
C ₄ H ₆ O ₃ [CH ₃ CH(CO ₃)CH ₂]	Propylene carbonate	T. Kinjo Y. Kawashima E. Hirota ^a	Normal, ¹³ C (4 species), ¹⁸ O (3 species) assigned.
C ₄ H ₇ NO ₂ [(CH ₃ CO) ₂ NH]	Diacetamide	Y. Kawashima R. D. Suenram ^b E. Hirota ^a	<i>A</i> state and <i>E</i> state assigned.
C ₄ H ₈ N ₂ O ₂ [CH ₃ CONHCH ₂ CONH ₂]	<i>N</i> _α -Acetylglycinamide	Y. Kawashima R. J. Lavrich ^d R. D. Suenram ^b E. Hirota ^a	<i>A</i> state assigned, <i>E</i> state assignment in progress.
C ₄ H ₉ NO [CH ₃ CONHCH ₂ CH ₃]	<i>N</i> -Ethylacetamide	T. Usami K. Ohba Y. Kawashima R. D. Suenram ^b E. Hirota ^a	Manuscript prepared.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₁₀ O [CH ₃ CH ₂ CH ₂ CH ₂ OH]	<i>n</i> -Butanol	T. Uzuyama Y. Kawashima E. Hirota ^a	Seven rotamers assigned.
C ₄ H ₁₀ O [CH(CH ₃) ₂ CH ₂ OH]	Isobutanol	T. Uzuyama Y. Kawashima E. Hirota ^a	Four rotamers assigned.
C ₄ H ₁₀ S [CH ₃ CH ₂ CH ₂ CH ₂ SH]	<i>n</i> -Butanethiol	Y. Tanaka Y. Kawashima E. Hirota ^a	Seven rotamers, one for SD assigned.
C ₄ H ₁₀ S [CH(CH ₃) ₂ CH ₂ SH]	Isobutanethiol	Y. Tanaka Y. Kawashima E. Hirota ^a	Three rotamers, ³⁴ S, ¹³ C species assigned.
C ₅ H ₁₀ O [<u>CH₂CH₂CH₂CH₂CHOH</u>]	Cyclopentanol	Y. Kawashima E. Hirota ^a B. Carroll ^f G. Blake ^f	Work in progress
C ₅ H ₁₂ O [CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ OH]	<i>n</i> -pentanol	Y. Kawashima Y. Komamine E. Hirota ^a	Six isomers assigned.
C ₅ H ₁₂ O [H ₃ CCH ₂ CH(CH ₃)CH ₂ OH]	2-Methyl-1-butanol	Y. Kawashima N. Koshimae Y. Tanimoto E. Hirota ^a	Three conformers assigned.
C ₅ H ₁₂ S [(CH ₃) ₃ CSCH ₃]	<i>Tert</i> -butyl methyl sulfide	Y. Kawashima R. Watanabe E. Hirota ^a	Normal, ³⁴ S, ¹³ C species assigned.
C ₆ H ₆ O [(HCCCH ₂) ₂ O]	Dipropargyl ether	T. Usami Y. Kawashima	Work almost completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₆ S [C ₆ H ₅ SH]	Thiophenol	R. Jono ^e A. Hino ^e M. Onda ^e Y. Kawashima	Normal, D, ³⁴ S, ¹³ C species assigned
C ₆ H ₁₀ [CH=CHCH ₂ CH ₂ CH ₂ CH ₂]	Cyclohexene	Y. Kawashima E. Hirota ^a	Isotopomer assigned.
C ₆ H ₁₀ O [CH ₃ CH ₂ CH ₂ CH=CHCHO]	<i>Trans</i> -2-hexenal	R. Yokoyama Y. Kawashima E. Hirota ^a	Four conformers assigned
C ₆ H ₁₀ O ₂ [O(CO)CH ₂ CH ₂ CH(CH ₂ CH ₃)]	γ-Hexanolactone	T. Takimoto ^e N. Kuze ^e Y. Kawashima	Three conformers assigned
C ₆ H ₁₄ O [CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ OH]	<i>n</i> -Hexanol	Y. Hosoya Y. Kawashima E. Hirota ^a	Three conformers assigned
C ₈ H ₁₂ [CH=CHCH ₂ CH(CH=CH ₂)CH ₂ CH ₂]	4-Vinyl-1-cyclohexene	Y. Nakanishi Y. Kawashima R. J. Lavrich ^d R. D. Suenram ^b E. Hirota ^a	Two conformers assigned.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
BrH ₃ O (H ₂ O...HBr)	Water...hydrogen bromide	BP, OD, LP, ZK, <i>Bri</i>	FTMW: isotopic work+dipole moment - completed, ms. in prep.
Cl ₂ H ₆ O ₂ ((H ₂ O) ₂ (HCl) ₂)	Water...hydrogen chloride (2/2)	<i>Vir</i> , ZK	Assigned in chirped pulse FTMW, ms. in prep.
ClH ₇ O ₃ ((H ₂ O) ₃ HCl)	Water...hydrogen chloride (3/1)	<i>Vir</i> , ZK	Assigned in chirped pulse FTMW, ms in prep.
H ₁₂ O ₆ (H ₂ O) ₆)	Water hexamer	<i>Vir</i> , ZK	All 64 combinations of ¹⁶ O/ ¹⁸ O for each of three hexamer conformers observed and analysed.
FH ₃ O (H ₂ O...HF))	Water...hydrogen fluoride	ZK, <i>NN</i>	MMW spectrum, new analysis
ArClH ₃ O ((H ₂ O...HCl)...Ar)	(Water...hydrogen chloride)...argon	EBJ, ZK, LP, <i>Vir</i>	FTMW (Balle-Flygare and chirped pulse): parent+D+ ³⁷ Cl+ ¹⁸ O, dipole moment, ms in prep.
CH ₄ N ₂ O (NH ₂) ₂ C=O	Urea	<i>Koln</i> , <i>Wri</i> , ZK	Astrophysical detection submitted, lab spectroscopy g.s.+e.s., in prep.
C ₄ H ₇ Cl (C ₄ H ₆ ...HCl)	1,3-butadiene...hydrogen chloride	ZK, <i>Bri</i>	FTMW: partial assignment
C ₅ H ₈ N ₂ O	2-aminopyridine... H ₂ O cyclic dimer	AK, EBJ, ZK, LP, <i>Rennes</i>	FTMW: nearing completion, more isotopic species measured
C ₂ Cl ₃ N (Cl ₃ CCN)	Trichloroacetonitrile	ZK, LP, EBJ	FTMW: hyperfine from 4 nuclei resolved and fitted
C ₂ Cl ₃ F ₃ (Cl ₃ CCF ₃)	CFC-113a	<i>Bilbao</i> , LP, EBJ, ZK	Chirped pulse+cavity FTMW, MMW
C ₂ Cl ₄ F ₂ (Cl ₃ CCClF ₂)	CFC-112a	<i>Bilbao</i> , EBJ, ZK	Chirped pulse+cavity FTMW, <i>JMS</i> 352 ,1(2018).
C ₂ H ₃ NO (CH ₃ NCO)	Methyl isocyanate	<i>Val</i> , <i>Rennes</i> , ZK	Both single ¹³ C species assigned in enriched spectra, <i>K_a</i> >3 transitions for the parent. ms in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₃ NS (CH ₃ NCS)	Methyl isothiocyanate	Ohio, ZK	FASSST spectrum partially analysed
C ₂ H ₆ N ₂ O (H ₂ NCH ₂ CONH ₂)	Glycine amide	ZK, LP, Rennes, Val	Ablation+supersonic expansion FTMW: part I, <i>ApJ</i> 861 ,70(2018); MMW, inversion, vibr.satellites: part II in prep.
C ₂ H ₇ N (C ₂ H ₅ NH ₂)	Ethylamine	Ohio, AK, ZK, Koln	Spectrum up to 1 THz, torsion + inversion analysis in prog.
C ₃ H ₈ O ₄ , C ₃ H ₁₀ O ₅ , C ₃ H ₁₂ O ₆	LacticAcid+H ₂ O LacticAcid+(H ₂ O) ₂ LacticAcid+ (H ₂ O) ₃	Vir, ZK,EBJ	Chirped pulse FTMW: clusters of lactic acid with H ₂ O and two lactide conformers, ms. in prep.
C ₆ H ₈ O ₄	Lactide		
C ₃ H ₈ O (CH ₃ CH ₂ CH ₂ OH)	<i>n</i> -propanol	ZK, Ohio, JPL	<i>T</i> series of conformers: in progress
CH ₂ Cl ₂ C ₃ H ₂ ClN C ₄ H ₄ N ₂	Methylene chloride 2-chloroacrylonitrile Pyrimidine	OD, ZK, Bold	FTMW: dipole moment from Stark effect under resolved hfs from two quadrupolar nuclei
C ₅ H ₆ N ₂	2-Aminopyridine	ZK, LP	MMW+FTMW: c.d., hyperfine, g.s. + inversion satellite
C ₅ H ₈	Isoprene	ZK, LP, JPL, Par, Har	MMW+FTMW+FTIR: parent+satellites, ms in prep.
C ₅ H ₁₂ O ((CH ₃) ₃ CCH ₂ OH)	Neopentyl alcohol	LP, ZK, Goet	MMW+FTMW: two conformers assigned
C ₆ H ₄ Cl ₂	1,2-dichlorobenzene	ZK, LP, EBJ	Chirped pulse FTMW+MMW, g.s.+vibrational satellites+structure
C ₆ H ₅ F	Fluorobenzene	ZK, EBJ	WG-FTMW in CMW region, submitted; further vibr. states in prog.
C ₇ H ₅ N	Benzonitrile	Wisc, ZK	g.s.+e.s., MMW: <i>JMS</i> 352 ,1(2018). Higher vibr. states in prog.
C ₇ H ₇ Cl	<i>p</i> -chlorotoluene	Kha, Han, ZK,	Low-barrier sixfold internal rotation with hyperfine, in prog.
C ₈ H ₇ N	<i>p</i> -Cyanotoluene	EBJ, ZK, LP	MMW+FTMW: c.d. + internal rot., in progress
C ₁₀ H ₁₆ O,	Thujone	Hamb, ZK	Chirped pulse FTMW, heavy atom molecular backbones from ¹³ C and ¹⁸ O in natural abundance.
C ₁₀ H ₁₈ O ₂ , C ₁₀ H ₂₀ O ₃	Thujone+H ₂ O Thujone+(H ₂ O) ₂		Several cluster conformers assigned.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₁₀ H ₁₅ F C ₁₀ H ₁₅ Cl C ₁₀ H ₁₅ Br C ₁₀ H ₁₅ I	1-fluoro-adamantane 1-chloro-adamantane 1-bromo-adamantane 1-iodo-adamantane	BP, ZK, LP, <i>Bri</i>	MMW + FTMW, electric dipole moment, completed
CINO ₃ (CIONO ₂)	Chlorine nitrate	<i>Ohio</i> , ZK, EBJ	FASSST spectrum: further vibrational satellites in prog.
HN ₃	Hydrazoic acid	<i>Pra</i> , <i>Wisc</i> , ZK	Broadband MMW+SMM: analysis of higher states in prog.

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A database "Programs for Rotational Spectroscopy (PROSPE)" is available at:

<http://info.ifpan.edu.pl/~kisiel/prospe.htm>

A new database on "History of Rotational Spectroscopy" is being constructed at:

<http://info.ifpan.edu.pl/~kisiel/rothist/rothist.html>

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH ₄ O (CH ₃ OH, ¹³ CH ₃ OH CH ₃ ¹⁸ OH, CH ₃ OD)	Methanol	F. Matsushima K. Kobayashi	ground and CO stretching vibrational state, far infrared spectrum and Zeeman effect
CH ₄ S (CH ₃ SH, CD ₃ SH)	Methanethiol	K. Kobayashi	mm-wave spectrum 1st and 2nd excited torsional states assigned
CH ₅ N (CH ₃ NH ₂)	Methylamine	K. Kobayashi	mm-wave spectrum prep. spectrum atlas
C ₂ H ₄ O ₂ (HCOOCH ₃ , DCOOCH ₃ , H ¹³ COOCH ₃ HCOO ¹³ CH ₃)	Methyl formate	K. Kobayashi ^{1,2}	HCOOCH ₃ , two new vibrational states assigned Infrared spectrum
C ₂ H ₆ O (C ₂ H ₅ OH)	Ethanol	K. Kobayashi	spectrum assigned
C ₂ O (¹³ CCO, C ¹³ CO, ¹³ C ¹³ CO, CC ¹⁸ O)	Ketenylidene	K. Kobayashi ³	Normal species extended to 715 GHz spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₃ H ₃ NO	Isoxazole Oxazole	K. Kobayashi	ground state assigned in preparation of the manuscript
C ₃ H ₃ NS	Isothiazole	K. Kobayashi	ground state assigned
C ₃ H ₅ N (CH ₃ CH ₂ CN)	Ethyl cyanide	Y. Fukuyama ⁴ K. Kobayashi H. Odashima ⁵	prep. spectrum atlas
C ₃ H ₆ O ₂ (CH ₃ COOCH ₃)	Methyl Acetate	K. Kobayashi ⁶ I. Kleiner ⁷	mm-wave spectrum
C ₃ H ₈ O (CH ₃ OC ₂ H ₅)	Ethyl methyl ether	K. Kobayashi ^{1,2}	mm-wave spectrum ground and excited states assigned (skeletal torsion vt=2,3)
C ₄ H ₄ S	Thiophene	K. Kobayashi	40-170 GHz spectrum assigned
H ₂ N (NHD)	Amidogen	K. Kobayashi ⁸	Terahertz spectra in preparation of the manuscript

1. In collaboration with M. Fujitake (Kanazawa University, Japan).
2. In collaboration with N. Ohashi (Kanazawa University, Japan).
3. In collaboration with T. Furuya and S. Saito (Fukui University, Japan) for mm spectrum and with Y. Sumiyoshi and Y. Endo (University of Tokyo, Japan) for FT mw spectrum.
4. SPring-8/JASRI, Sayo-cho, Sayo-gun, Hyogo, 679-5148, Japan.
5. Department of Physics, Meiji University, Mita Kawasaki 214-8571, Japan.
6. In collaboration with S. Shipman (New College of Florida, USA).
7. Laboratoire Interuniversitaire des Systemes Atmospheriques (LISA), Creteil, France.
8. In collaboration with H. Ozeki (Toho University, Japan)

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAMES OF INVESTIGATORS</u>	<u>PRESENT STAGE OF PROGRESS</u>
C₂H₆N₂O₆	Formamidinium Formate	Z, Zhou, R. Aitken, C. Cardinaud, A. Slawin, H. Wang, A. Daly, M. Palmer, S. Kukolich	<i>J. Chem. Phys.</i> 150 , 094305 (2019)
C₆H₆BCl	1-Chloroborepin	A. M. Pejlovas, Z. Zhou, A. Ashe III, S. G. Kukolich	<i>J. Phys. Chem. A.</i> 122 (6) 1542-1549 (2018)
C₉H₆O₂	Phenylpropionic Acid	Aaron M. Pejlovas, Zunwu Zhou, Wei Lin, Stephen G. Kukolich	<i>J. Mol. Spectrosc.</i> 338 , 1-3 (2018)
C₄HNO₂	H – C ≡ C – C ≡ N · · O=C=O	L. Kang, P. Davis, I. Dorell, K. Li, O. Oncer, L. Wang, S. E. Novick, S. G. Kukolich	<i>J. Mol. Spectrosc.</i> 342 , 62-72 (2017)
C₁₀H₈O₄	Phenylpropionic Acid – Formic Acid Dimer	Aaron M. Pejlovas, Zunwu Zhou, Wei Lin, Stephen G. Kukolich	Scanning in progress
C₆H₃MnO₅	Methyl manganese pentacarbonyl	Z. Z. Zhou, A. M. Pejlovas S. G. Kukolich	Scanning in progress
C₁₂H₁₂FeO₄	Ferrocenecarboxylic acid – formic acid dimer	A. M. Pejlovas Z. Z. Zhou, S.G. Kukolich	Scanning in progress
C₁₀H₈O₄	Phenylpropionic Acid – Formic Acid Dimer	A. M. Pejlovas, Z. Zhou, Wei Lin, Stephen G. Kukolich	Scanning in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAMES OF INVESTIGATORS</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{11}H_{10}FeO_2$	Ferrocenecarboxylic acid	A. M. Pejlovas, Z. Z. Zhou S. G. Kukolich	<i>J. Mol. Spectrosc.</i> 338 , 77-80 (2017)

Name to whom queries should be addressed: Nobuhiko Kuze, Yoshiyuki Kawashima

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CF ₂ NOPS (F ₂ P(S)-NCO)	Difluorothiophosphoryl isocyanate	S. Watanabe N. Kuze	Spectrum assigned.
CF ₂ NPS ₂ (F ₂ P(S)-NCS)	Difluorothiophosphoryl isothiocyanate	S. Watanabe N. Kuze	Spectrum assigned.
C ₂ H ₃ N ₃ O ₂ (CH ₃ OC(=O)N ₃)	Methyl azidoformate	S. Watanabe N. Kuze	Spectrum assigned.
C ₃ H ₃ NO ₃ (CH ₃ OC(=O)NCO)	Methoxycarbonyl isocyanate	S. Watanabe N. Kuze	Manuscript in prep.
C ₃ H ₅ NO (CH ₃ CH ₂ -OCN)	Ethyl cyanate	T. Sakaizumi N. Kuze	Manuscript in prep.
C ₃ H ₅ NO (CH ₃ CH=CH-NO)	1-Nitrosopropene	T. Sakaizumi N. Kuze	ν_3 ($\nu=1$) determined. Manuscript in prep.
C ₄ H ₇ NO (HNCH ₂ (CH ₂) ₂ C=O)	2-Pyrrolidone	N. Kuze	Manuscript in prep.
C ₄ H ₇ NO (CH ₂ (CH ₂) ₂ C=NOH)	Cyclobutanone oxime	E. Sato N. Kuze	Manuscript in prep.
C ₄ H ₉ NO (CH ₃ (CH ₂) ₂ CH=NOH)	(Z)-n-Butyraldehyde oxime	O. Ohashi N. Kuze	Observation of hyper- fine structure
C ₆ H ₁₁ NO (HNCH ₂ (CH ₂) ₄ C=O)	ϵ -Caprolactam	N. Kuze	Manuscript in prep.
C ₆ H ₁₂ O ₂ (CH ₃) ₃ C(=O)COCH ₃)	Methyl Trimethylacetate	N. Kuze	Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_6H_{11}NO$ $(OC(=O)(CH_2)_2CH-C_2H_5)$	γ -Hexanolactone	T. Takimoto	Spectrum assigned.
$C_9H_{10}O_2$ $(C_6H_5CH_2OCOCH_3)$	Benzyl acetate	N. Kuze	Spectrum obsd.

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(Entries marked with * are collaborative studies between this laboratory and that of N. R. Walker, School of Chemistry, Bedson Building, Newcastle University, Newcastle-upon-Tyne, NE1 7RU, UK)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
AuH ₃ IN*	H ₃ N...Au-I	D. Bittner, S.L. Stephens	Spectrum assigned.
BrH ₃ O	H ₂ O...H-Br	A. P. Suckley	Published: <i>Chem. Phys. Lett.</i> , 150 , 153 (1988). Further work with Z. Kisiel.
CClFPt*	FCPtCl	D. Bittner, G. Cooper, C. Medcraft	Spectra of isotopologues assigned.
CF ₂ Pt*	FCPtF	D. Bittner, G. Cooper, C. Medcraft	Spectra of isotopologues assigned.
CH ₃ F ₃ IP*	H ₃ P...I-CF ₃	S. L. Stephens	Spectrum assigned.
CH ₃ NS ₂ *	H ₃ N...S=C=S	E. Gougoula, C Medcraft	<i>J. Chem. Phys.</i> , in press
CH ₄ ArN ₂ O*	Urea...Ar	C. Medcraft	Spectrum assigned
CH ₄ ArN ₂ S*	Thiourea...Ar	C. Medcraft	Spectrum assigned
CH ₄ ClF	CH ₄ ...Cl-F	D.G. Lister	Spectrum assigned.
CH ₅ F	CH ₄ ...H-F	D.G. Lister	With F.J. Lovas at NIST. Isotopic work complete.
CH ₆ N ₂ OS*	Thiourea...H ₂ O	C. Medcraft	Spectrum assigned.
C ₂ H ₂ AgI*	C ₂ H ₂ ...Ag-I	S. L. Stephens	Spectrum assigned.
C ₂ H ₂ CuF*	C ₂ H ₂ ...Cu-F	S. L. Stephens, D. P. Zaleski	Spectrum assigned, isotopic work
C ₂ H ₂ CuI	C ₂ H ₂ ...Cu-I	S. L. Stephens, D Bittner	Spectrum assigned.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₄ AgF*	C ₂ H ₄ ···Ag-F	S. L. Stephens	Spectrum assigned.
C ₂ H ₄ AgI*	C ₂ H ₄ ···Ag-I	S. L. Stephens	Spectrum assigned.
C ₂ H ₄ AuI*	C ₂ H ₄ ···Au-I	S. L. Stephens, M. Sprawling, D. P. Zaleski	Spectra of isotopologues assigned.
C ₂ H ₄ CuF*	C ₂ H ₄ ···Cu-F	S. L. Stephens	Spectrum assigned.
C ₂ H ₄ CuI*	C ₂ H ₄ ···Cu-I	S. L. Stephens	Spectrum assigned.
C ₂ H ₅ BrS	(CH ₂) ₂ S···H-Br	S. Batten	¹³ C and ³⁴ S species assigned.
C ₃ H ₂ F ₃ I*	C ₂ H ₂ ···ICF ₃	S. L. Stephens	Manuscript in preparation
C ₃ H ₉ AgIN*	(CH ₃) ₃ N···Ag-I	D. Bittner, S. L. Stephens	Spectrum assigned. Manuscript in preparation.
C ₃ H ₉ F ₆ NS*	(CH ₃) ₃ N···SF ₆	D. Bittner	Spectrum assigned.
C ₄ H ₆ O	(CH ₂) ₂ O···HC≡CH	S. Batten	All singly substituted ¹³ C species assigned.
C ₄ H ₈ N ₄ O*	Urea···imidazole	S. Blanco (Valladolid), J. C. Mullaney, C. Medcraft	Spectrum assigned, isotopic work.
C ₄ H ₉ NS ₂ *	(CH ₃) ₃ N···S=C=S	E. Gougoula, C. Medcraft	Manuscript in preparation
FIPt*	FPI	D. Bittner, G. Cooper, C. Medcraft	Spectra of isotopologues assigned.
H ₃ IS	H ₂ S···H-I	A. P. Suckley	Spectrum assigned. Further work.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₄ OS (CH ₃ COSH)	Thioacetic Acid	C.J. Smith A. K. Huff H. Zhang Y. Mo K.R. Leopold	<i>J. Chem. Phys.</i> , in press Internal rotation in two conformers
C ₂ HF ₃ O ₅ S (CF ₃ COOSO ₂ OH)	Trifluoroacetic Sulfuric Anhydride	A.K. Huff C. J. Smith R.B. Mackenzie K.R. Leopold	<i>J. Phys. Chem. A.</i> , in press DOI 10.1021/acs.jpca.9b00300
C ₂ H ₆ O ₆ S (CH ₃ COOSO ₂ OH–H ₂ O)	Acetic sulfuric anhydride – H ₂ O complex	C.J. Smith A.K. Huff R.B. Mackenzie K.R. Leopold	<i>J. Phys. Chem. A</i> 2018 , 122, 4549 – 4554.
CH ₃ ArI (Ar–CH ₃ I)	Argon – methyl iodide complex	A.K. Huff C.J. Smith K.R. Leopold	<i>J. Mol. Spectrosc.</i> 2018 , 353, 6-10.
C ₃ H ₂ O ₅ S (HC≡C–COOSO ₂ OH)	Propiolic sulfuric anhydride	C.J. Smith A. Huff R.B. Mackenzie K.R. Leopold	Three isotopologues observed and analyzed; statistical thermodynamics; manuscript in preparation.
CHF ₃ O ₃ S CF ₃ SO ₂ OH	Triflic Acid	A.K. Huff C.J. Smith N. Love K. R. Leopold	Manuscript in preparation
CH ₃ F ₃ O ₄ S CF ₃ SO ₂ OH–H ₂ O	Triflic acid – water complex	A.K. Huff K.R. Leopold	Three isotopologues manuscript in preparation
CH ₅ F ₃ O ₅ S CF ₃ SO ₂ OH–(H ₂ O) ₂	Triflic acid – (H ₂ O) ₂ complex	A.K. Huff K.R. Leopold	Assignments in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_4F_6O_3$ ($CF_3COOCOCF_3$)	Trifluoroacetic acid anhydride	N. Love C.J. Smith K.R. Leopold	manuscript in preparation
$C_2H_6O_2S$ ($CH_3COSH-H_2O$)	Thioacetic acid – water complex	A.K. Huff C.J. Smith K.R. Leopold	Three isotopologues manuscript in preparation
O_5S_2 SO_3-SO_2	SO_3-SO_2 complex	R.B. Mackenzie A.K. Huff K.R. Leopold	Manuscript in preparation.
C_5H_7NO (pyridine – water)	pyridine – water complex (HOD)	R.B. Mackenzie C.T. Dewberry C.J. Smith R.D. Corneilus K.R. Leopold	Spectra assigned and fit for both HOD and DOH species.
$C_7H_5F_2N$ (2,6-difluoropyridine-HCCH)	2,6-difluoropyridine-HCCH complex	C.T. Dewberry R.B. Mackenzie K.R. Leopold	HCCH, DCCD, and HCCD isotopologues; Manuscript in preparation.
$C_6H_5NS_2$ (pyridine- CS_2)	$C_5H_5N-CS_2$ (pyridine- CS_2 complex)	B. Timp, S. Iyer, K.R. Leopold	Spectra observed.
$C_3H_9ArO_3NS$	$(CH_3)_3N-SO_3-Ar$ complex	C.T. Dewberry R.B. Mackenzie B.A. Timp K.R. Leopold	Spectra observed.
$C_2H_6O_3$ ($C_2H_6O_3-H_2O$)	acetic acid - water complex	G. Sedo S. Wu K.R. Leopold	Spectra assigned and fit $CH_3COOH-^{13}CH_3$ Internal rotation barrier determined.
$ArHNO_3$ (HNO_3-Ar)	nitric acid – argon complex	J.L. Doran G. Sedo K.R. Leopold	Spectrum observed, rotational assignments.
$C_5H_{11}N_3$ ($(CH_3)_3N-HCN-HCN$)	$(CH_3)_3N-HCN-HCN$ complex	M. Craddock C.S. Brauer K.R. Leopold	11 isotopologues assigned and analyzed.
$C_3H_{11}F_2N$ ($(CH_3)_3N-HF-HF$)	$(CH_3)_3N-HF-HF$ complex	C.S. Brauer M. Craddock G. Sedo S. W. Hunt K.R. Leopold	8 isotopologues assigned and analyzed Manuscript in preparation.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_7H_6O_2$ ($CO_2-C_6H_6$)	CO_2 -Benzene complex	J.L. Doran K.R. Leopold	Spectrum observed; not assigned.
BF_3H_2O (H_2O-BF_3)	H_2O-BF_3 complex	D.L. Fiacco S.W. Hunt K. J. Higgins M.E. Ott K.R. Leopold	6 isotopologues observed; Internal motion
CH_3BF_4 (CH_3F-BF_3)	methyl fluoride- BF_3 complex	J.A. Phillips M. Canagaratna M.E. Ott K.R. Leopold	Spectra observed for ^{10}B and ^{11}B species with CH_3F and $^{13}CH_3F$; two internal rotor states.
$C_6H_{18}GaN$ $N(CH_3)_3$ complex	$(CH_3)_3Ga-N(CH_3)_3$	S.W. Hunt D.L. Fiacco K.R. Leopold	^{14}N and ^{15}N species $(CH_3)_3Ga$ -observed.
ClH_2NO_3 ($HCl-HNO_3$)	HCl -nitric acid complex	M.E. Ott K.R. Leopold	a-type spectrum for ^{35}Cl , ^{37}Cl , ^{14}N , and ^{15}N and DNO_3 species.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₆ F ₄ S ₃ (C ₂ F ₄ S ₂ ... C ₂ H ₆ S)	2,2,4,4-Tetrafluoro-1,3-dithiethane ... dimethylsulfide	Obenchain ^a , Juanes, Spada ^b , Grabow ^a , Lesarri	Assigned
C ₄ H ₁₂ S ₂ (C ₂ H ₆ S) ₂	Ethane thiol dimer	Zhang ^c , Li ^c , Gou ^c , Feng ^c , Lesarri	Assigned
C ₅ H ₆ OS	Thenyl alcohol	Juanes, Saragi, Lesarri	Assigned
C ₅ H ₆ S ₂	Thenyl mercaptan	Juanes, Saragi, Lesarri	Assigned
C ₅ H ₇ NO	Furfuryl amine	Juanes, Lesarri	Assigned
C ₅ H ₇ NS	Thenyl amine	Juanes, Lesarri	Assigned
C ₅ H ₁₃ NO ₂	2-aminopentane-1,3-diol	Uriarte ^d , Cocinero ^d , Lesarri	In preparation
C ₅ H ₈ O ₃ (C ₅ H ₆ O ₂ ... H ₂ O)	Furfuryl alcohol ... H ₂ O	Juanes, Lesarri	CEJ, 2018, 24, 6564
C ₅ H ₈ O ₂ S (C ₅ H ₆ OS ... H ₂ O)	Furfuryl mercaptan ... H ₂ O	Juanes, Lesarri	CEJ, 2018, 24, 6564
C ₅ H ₈ O ₂ S (C ₅ H ₆ OS ... H ₂ O)	Thenyl alcohol ... H ₂ O	Juanes, Saragi, Lesarri	In preparation
C ₅ H ₈ OS ₂ (C ₅ H ₆ S ₂ ... H ₂ O)	Thenyl mercaptan ... H ₂ O	Juanes, Saragi, Lesarri	In preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₅ H ₅ F ₃ O ₂ (C ₄ H ₃ F ₃ O ... H ₂ C=O)	Trifluoroacetone... Formaldehyde	Pérez ^e , Lesarri, Jahn ^a , Dewald ^a , Grabow ^a	Analysis in progress
C ₆ H ₈ OS	2-Thiopheneethanol	Juanes, Lesarri	Assigned
C ₆ H ₈ OS	3-Thiopheneethanol	Juanes, Lesarri	Assigned
C ₆ H ₂ F ₅ NO (C ₅ F ₅ N ... H ₂ C=O)	Pentafluoropyridine ... Formaldehyde	Gou ^c , Feng ^c , Juanes, Lesarri	Spectrum recorded
C ₆ H ₁₂ O	Cyclohexanol	Juanes, Li ^f , Spada ^b , Evangelisti ^f , Lesarri, Caminati ^f	<i>PCCP</i> , 2019, 21, 3676
C ₆ H ₁₂ S	Cyclohexanethiol	Juanes, Lesarri, Evangelisti ^f ,	Assigned
C ₆ H ₁₃ N	Cyclohexylamine	Juanes, Lesarri,	Assigned
C ₆ H ₁₄ O ₂ (C ₆ H ₁₂ O ... H ₂ O)	Cyclohexanol ... H ₂ O	Juanes, Li ^f , Spada ^b , Evangelisti ^f , Lesarri, Caminati ^f	<i>PCCP</i> , 2019, 21, 3676
C ₆ H ₁₄ O ₂ S (C ₆ H ₁₂ S ... H ₂ O)	Cyclohexanethiol ... H ₂ O	Juanes, Lesarri, Evangelisti ^f	Assigned
C ₆ H ₁₅ NO (C ₆ H ₁₃ N ... H ₂ O)	Cyclohexylamine ... H ₂ O	Juanes, Lesarri,	Assigned
C ₆ H ₆ N ₂ O (C ₅ NH ₄ CONH ₂)	Nicotinamide	Caminati ^f , Cocinero ^d , Lesarri	In preparation
C ₆ H ₁₀ S ₂	Diallyl disulfide	Saragi, Juanes, Lesarri	In preparation
C ₆ H ₁₁ NO	ε-Caprolactam	Wachsmuth ^a , Vallejo, Lesarri, Grabow ^a	Assigned
C ₆ H ₁₂ O	Oxepane	Borter ^a , Wachsmuth ^a , Lesarri, Cocinero ^d , Grabow ^a	Assigned
C ₆ H ₁₃ N	Azepane	Wachsmuth ^a , Vallejo, Grabow ^a , Lesarri,	Assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₇ H ₆ F ₂	2,3-difluorotoluene	Nair ^a , Herbers ^a , Grabow, Lesarri	<i>JMS</i> , 2018, 349, 37
C ₇ H ₆ F ₂	2,4-difluorotoluene	Nair ^a , Herbers ^a , Obenchain ^a , Grabow ^a	<i>JMS</i> , 2018, 344, 21
C ₇ H ₇ Cl	Meta-chlorotoluene	Nair ^a , Herbers ^a , Grabow Lesarri	<i>JMS</i> , 2019, In press
C ₇ H ₈ S	Benzyl mercaptan	Saragi, Lesarri, Caminati ^l	In preparation
C ₇ H ₁₂	Ethynylcyclohexane	Vogt ^g , Demaison ^g , Rudolph ^g , Juanes, Fernández, Lesarri	<i>JCP</i> , 2018, 148, 064306
C ₇ H ₁₃ Cl	Chlorocycloheptane	Juanes, Lesarri	Assigned
C ₇ H ₁₀ O ₂ (C ₇ H ₈ O ... H ₂ O)	Benzyl alcohol ... H ₂ O	Saragi, Lesarri	Assigned
C ₇ H ₁₂ O ₃ (C ₇ H ₈ O ... 2 H ₂ O)	Benzyl alcohol ... 2H ₂ O	Saragi, Lesarri	Assigned
C ₇ H ₁₀ OS (C ₇ H ₈ S ... H ₂ O)	Benzyl mercaptan ... H ₂ O	Saragi, Lesarri	Assigned
C ₈ H ₁₀ S	Phenylethyl mercaptan	Saragi, Lesarri	Assigned
C ₈ H ₁₂ N	Cyanocycloheptane	Wachsmuth ^a , Lesarri Grabow ^a	In preparation
C ₈ H ₁₂ O ₂ (C ₈ H ₁₀ O ... H ₂ O)	Phenyl ethyl alcohol ... H ₂ O	Saragi, Lesarri	Assigned
C ₈ H ₁₂ OS (C ₈ H ₁₀ S ... H ₂ O)	Phenylethyl mercaptan ... H ₂ O	Saragi, Lesarri	Assigned
C ₉ H ₁₃ NO ₃ (C ₉ H ₁₁ NO ₂ ...H ₂ O)	Benzocaine ... H ₂ O	Lesarri, Shipman ^h , Pate ⁱ	Assigned
C ₁₀ H ₁₂ O ₄ (C ₅ H ₆ O ₂) ₂	Furfuryl alcohol dimer	Juanes, Saragi, Lesarri	In preparation
C ₁₀ H ₁₂ O ₂ S ₂ (C ₅ H ₆ OS) ₂	Thenyl alcohol dimer	Juanes, Saragi, Lesarri	In preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₁₀ H ₁₂ O ₃ (HO C ₆ H ₃ (OCH ₃)C ₂ H ₂ CH ₂ OH)	Coniferyl alcohol	Cocinero ^d , Lesarri	In preparation
C ₁₀ H ₁₄ O ₃ (HO C ₆ H ₃ CH ₂ CH ₂ CH(CO)CH ₃)	Zingerone	Cocinero ^d , Lesarri, Caminati ^f	In preparation
C ₁₁ H ₁₅ NO ₂ (NH ₂ C ₆ H ₄ COO(CH ₂) ₃ CH ₃)	Butamben	Lesarri, Cocinero ^d , Caminati ^f , Grabow ^a	In preparation
C ₁₁ H ₁₅ NO ₂ (NH ₂ C ₆ H ₄ COOCH ₂ CH(CH ₃) ₂)	Isobutamben	Lesarri, Cocinero ^d	In preparation
C ₁₂ H ₁₂ S ₂ (C ₆ H ₆ S) ₂	Thiophenol dimer	Saragi, Lesarri	Assigned
C ₁₂ H ₁₆ O ₂ S ₂ (C ₆ H ₈ OS) ₂	2-Thiopheneethanol Dimer	Juanes, Lesarri	In preparation
C ₁₂ H ₁₆ O ₂ S ₂ (C ₆ H ₈ OS) ₂	3-Thiopheneethanol Dimer	Juanes, Lesarri	In preparation
C ₁₂ H ₂₄ O ₂ (C ₆ H ₁₂ O) ₂	Cyclohexanol dimer	Juanes, León, Lesarri	In preparation
C ₁₂ H ₂₆ N ₂ (C ₆ H ₁₃ N) ₂	Cyclohexyl amine dimer	Juanes, Lesarri	Assigned
C ₁₂ H ₁₀ S ₂	Diphenyl disulfide	Demaison ^g , Vogt ^g , Saragi, Juanes, Rudolph ^g , Lesarri	<i>CPC</i> , 2019, 20, 366
C ₁₂ H ₂₂ S ₂	Dicyclohexyl disulfide	Saragi, Juanes, Lesarri	Assigned
C ₁₂ H ₁₆ N ₂ O (C ₆ H ₇ N) ₂ ··· H ₂ O	Aniline dimer ··· H ₂ O	Pérez ^e , León, Lesarri	<i>ACIE</i> , 2018, 57, 15112
C ₁₄ H ₁₆ O ₂ (C ₇ H ₈ O) ₂	Benzyl alcohol dimer	Saragi, Lesarri	Assigned
C ₁₄ H ₁₆ S ₂ (C ₇ H ₈ S) ₂	Benzyl mercaptan dimer	Saragi, Lesarri	Assigned
C ₁₃ H ₁₁ O ₄ P	Phenyl saligenin phosphate	Juanes, Saragi, Lesarri	In preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{14}H_{13}O_4P$	Cresyl saligenin phosphate	Juanes, Saragi, Lesarri	In preparation
$C_{15}H_{24}N_2O$	Matrine	Juanes, Saragi, Lesarri	Assigned
$C_{16}H_{20}O_2$ ($C_8H_{10}O$) ₂	Phenylethyl alcohol dimer	Saragi, Lesarri	Assigned
$C_{16}H_{20}S_2$ ($C_8H_{10}S$) ₂	Phenylethyl mercaptan dimer	Saragi, Lesarri	Assigned
$C_{18}H_{21}N_3$ (C_6H_7N) ₃	Aniline trimer	Pérez ^e , León, Lesarri, Pate ⁱ , Martínez, Millán, Fernández	<i>ACIE</i> , 2018, 57, 15112

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
C ₂ HClF ₂ (<i>E</i>)-CF ³⁵ ClCHF, (<i>E</i>)-CF ³⁷ ClCHF, (<i>E</i>)- ¹³ CF ³⁵ ClCHF, (<i>E</i>)-CF ³⁵ Cl ¹³ CHF)	(<i>E</i>)-1-chloro- 1,2-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.
C ₂ H ₂ ClF ₃ (HF-(<i>E</i>)-CF ³⁵ ClCHF, HF-(<i>E</i>)-CF ³⁷ ClCHF, DF-(<i>E</i>)-CF ³⁵ ClCHF, DF-(<i>E</i>)-CF ³⁷ ClCHF)	hydrogen fluoride- (<i>E</i>)-1-chloro- 1,2-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.
C ₄ H ₃ ClF ₂ (HCCH-(<i>E</i>)-CF ³⁵ ClCHF, HCCH-(<i>E</i>)-CF ³⁷ ClCHF, H ¹³ CCH-(<i>E</i>)-CF ³⁵ ClCHF, HC ¹³ CH-(<i>E</i>)-CF ³⁵ ClCHF)	acetylene- (<i>E</i>)-1-chloro- 1,2-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.
C ₂ HArClF ₂ (Ar-(<i>E</i>)-CF ³⁵ ClCHF, Ar-(<i>E</i>)-CF ³⁷ ClCHF, Ar-(<i>E</i>)- ¹³ CF ³⁵ ClCHF, Ar-(<i>E</i>)-CF ³⁵ Cl ¹³ CHF)	argon-(<i>E</i>)-1-chloro- 1,2-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C ₂ H ₃ ClF ₂ (H ³⁵ Cl- <i>trans</i> -CHFCHF, H ³⁷ Cl- <i>trans</i> -CHFCHF)	hydrogen chloride- <i>trans</i> -1,2-difluoro- ethylene	Helen O. Leung Mark D. Marshall	J. Phys. Chem. A 122, 8363 (2018)
C ₂ H ₃ ClF ₂ (H ³⁵ Cl- <i>cis</i> -CHFCHF, H ³⁷ Cl- <i>cis</i> -CHFCHF, H ³⁵ Cl- <i>cis</i> - ¹³ CHFCHF)	hydrogen chloride- <i>cis</i> -1,2-difluoro- ethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
C ₄ H ₄ F ₂ (HCCH- <i>cis</i> -CHFCHF, H ¹³ CCH- <i>cis</i> -CHFCHF, HC ¹³ CH- <i>cis</i> -CHFCHF, HCCH- <i>cis</i> - ¹³ CHFCHF, HCCH- <i>cis</i> -CHF ¹³ CHF)	acetylene- <i>cis</i> -1,2-difluoro- ethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.
C ₄ H ₃ ClF ₂ (HCCH-CF ₂ CH ³⁵ Cl, HCCH-CF ₂ CH ³⁷ Cl, H ¹³ CCH-CF ₂ CH ³⁵ Cl, HC ¹³ CH-CF ₂ CH ³⁵ Cl)	acetylene-2-chloro- 1,1-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.
C ₂ H ₂ DF ₃ CHFCHF, DF- <i>cis</i> - ¹³ CHFCHF, DF- <i>cis</i> -CHF ¹³ CHF)	deuterium fluoride- <i>cis</i> -1,2-difluoro- ethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. (DF- <i>cis</i> -
C ₂ H ₃ ArCl (Ar-CH ₂ CH ³⁵ Cl, Ar-CH ₂ CH ³⁷ Cl)	argon-vinyl chloride	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C ₂ H ₄ Cl ₂ (H ³⁵ Cl-CH ₂ CH ³⁵ Cl, H ³⁵ Cl-CH ₂ CH ³⁷ Cl, H ³⁷ Cl-CH ₂ CH ³⁵ Cl)	hydrogen chloride- vinyl chloride	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C ₂ H ₃ Cl ₂ F (H ³⁵ Cl-(<i>Z</i>)-CHFCH ³⁵ Cl, H ³⁷ Cl-(<i>Z</i>)-CHFCH ³⁵ Cl, H ³⁵ Cl-(<i>Z</i>)-CHFCH ³⁷ Cl)	hydrogen chloride- (<i>Z</i>)-1-chloro-2- fluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C ₂ H ₂ ArClF (Ar-CH ₂ CF ³⁵ Cl, Ar-CH ₂ CF ³⁷ Cl)	argon-1-chloro- 1-fluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C ₂ H ₃ Cl ₂ F (H ³⁵ Cl-CH ₂ CF ³⁵ Cl, H ³⁵ Cl-CH ₂ CF ³⁷ Cl, H ³⁷ Cl-CH ₂ CF ³⁵ Cl)	hydrogen chloride- 1-chloro-1-fluoro- ethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C ₂ H ₂ Cl ₂ (CH ³⁵ ClCH ³⁵ Cl, CH ³⁵ ClCH ³⁷ Cl, CH ³⁷ ClCH ³⁷ Cl, CH ³⁵ Cl ¹³ CH ³⁵ Cl)	<i>cis</i> -1,2-dichloro- ethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
$C_2H_2ArCl_2$ ($Ar-CH^{35}ClCH^{35}Cl$, $Ar-CH^{35}ClCH^{37}Cl$)	argon- <i>cis</i> -1,2-dichloroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C_2H_2BrF ($CH_2C^{79}BrF$, $CH_2C^{81}BrF$)	1-bromo-1-fluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
$C_3H_3F_3O$ ($CH_2CH(CF_3)O$, $^{13}CH_2CH(CF_3)O$, $CH_2^{13}CH(CF_3)O$, $CH_2CH(^{13}CF_3)O$, $CH_2CH(CF_3)^{18}O$)	2-(trifluoromethyl)-oxirane	Helen O. Leung Mark D. Marshall	J. Phys. Chem. A 122, 4670 (2018)
$C_3H_3ArF_3O$ ($Ar-CH_2CH(CF_3)O$, $Ar-^{13}CH_2CH(CF_3)O$, $Ar-CH_2^{13}CH(CF_3)O$, $Ar-CH_2CH(^{13}CF_3)O$)	argon- 2-(trifluoromethyl)-oxirane	Helen O. Leung Mark D. Marshall	J. Phys. Chem. A 122, 4670 (2018)
$C_6H_6F_6O_2$ ($CH_2CH(CF_3)O-CH_2CH(CF_3)O$)	2-(trifluoromethyl)-oxirane dimer	Helen O. Leung Mark D. Marshall Nathan Seifert Yunjie Xu Wolfgang Jäger Anna Krin Sergio Domingos Melanie Schnell	Spectrum assigned. Manuscript in prep.
$C_{11}H_{11}F_3O_2$ ($CH_2CH(CF_3)O-CH_2CH(C_6H_5)O$)	2-(trifluoromethyl)-oxirane-styrene oxide	Helen O. Leung Mark D. Marshall Anna Krin Sergio Domingos Melanie Schnell	Spectrum assigned.
$C_3H_4F_2O$ ($CH_2CH(CHF_2)O$, $^{13}CH_2CH(CHF_2)O$, $CH_2^{13}CH(CHF_2)O$, $CH_2CH(^{13}CHF_2)O$, $CH_2CH(CHF_2)^{18}O$)	2-(difluoromethyl)-oxirane	Helen O. Leung Mark D. Marshall	J. Mol. Spectrosc. 350, 18 (2018)
$C_3H_4ArF_2O$ ($Ar-CH_2CH(CHF_2)O$)	argon- 2-(difluoromethyl)-oxirane	Helen O. Leung Mark D. Marshall	J. Mol. Spectrosc. 350, 18 (2018)
C_3H_5FO ($CH_2CH(CH_2F)O$, $^{13}CH_2CH(CH_2F)O$, $CH_2^{13}CH(CH_2F)O$, $CH_2CH(^{13}CH_2F)O$, $CH_2CH(CH_2F)^{18}O$)	2-(fluoromethyl)-oxirane	Helen O. Leung Mark D. Marshall	Spectrum assigned.

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
C_3H_5ArFO (Ar-CH ₂ CH(CH ₂ F)O)	argon- 2-(fluoromethyl)- oxirane	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C_4H_6O (CH ₂ CH(CHCH ₂)O, ¹³ CH ₂ CH(CHCH ₂)O, CH ₂ ¹³ CH(CHCH ₂)O, CH ₂ CH(¹³ CHCH ₂)O, CH ₂ CH(CH ¹³ CH ₂)O, CH ₂ CH(CHCH ₂) ¹⁸ O)	2-vinyloxirane	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C_4H_6ArO (Ar-CH ₂ CH(CHCH ₂)O)	argon-2-vinyloxirane	Helen O. Leung Mark D. Marshall	Spectrum assigned.
$C_3H_3ClF_4$ (H ³⁵ Cl-CH ₂ CF ₂ CF ₃)	hydrogen chloride- 2,3,3,3-tetrafluoro- propene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
$C_3H_2ClF_3$ (CH ₂ C ³⁵ ClCF ₃ , ¹³ CH ₂ C ³⁵ ClCF ₃ , CH ₂ ¹³ C ³⁵ ClCF ₃ , CH ₂ C ³⁵ Cl ¹³ CF ₃ , CH ₂ C ³⁷ ClCF ₃)	2-chloro-3,3,3- trifluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
$C_3H_2ArClF_3$ (Ar-CH ₂ C ³⁵ ClCF ₃ , Ar-CH ₂ C ³⁷ ClCF ₃)	argon-2-chloro- 3,3,3-trifluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
$C_3H_2ClF_3$ (<i>(Z)</i> -CH ³⁵ ClCHCF ₃ , (<i>Z</i>)- ¹³ CH ³⁵ ClCHCF ₃ , (<i>Z</i>)-CH ³⁵ Cl ¹³ CHCF ₃ , (<i>Z</i>)-CH ³⁵ ClCH ¹³ CF ₃ , (<i>Z</i>)-CH ³⁷ ClCHCF ₃)	(<i>Z</i>)-1-chloro- 3,3,3-trifluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
$C_3H_2ArClF_3$ (Ar-(<i>Z</i>)-CH ³⁵ ClCHCF ₃ , Ar-(<i>Z</i>)-CH ³⁷ ClCHCF ₃)	argon-(<i>Z</i>)-1-chloro- 3,3,3-trifluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
$C_3H_2ClF_3$ (<i>(E)</i> -CH ³⁵ ClCHCF ₃ , (<i>E</i>)- ¹³ CH ³⁵ ClCHCF ₃ , (<i>E</i>)-CH ³⁵ Cl ¹³ CHCF ₃ , (<i>E</i>)-CH ³⁵ ClCH ¹³ CF ₃ , (<i>E</i>)-CH ³⁷ ClCHCF ₃)	(<i>E</i>)-1-chloro- 3,3,3-trifluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₃ H ₂ ArClF ₃ (Ar-(<i>E</i>)-CH ³⁵ ClCHCF ₃ , Ar-(<i>E</i>)-CH ³⁷ ClCHCF ₃)	argon-(<i>E</i>)-1-chloro- 3,3,3-trifluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C ₃ H ₂ F ₄ ((<i>E</i>)-CHFCHCF ₃ , (<i>E</i>)- ¹³ CHFCHCF ₃ , (<i>E</i>)-CHF ¹³ CHCF ₃ , (<i>E</i>)-CHFCH ¹³ CF ₃)	(<i>E</i>)-1,3,3,3-tetra- fluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C ₃ H ₂ ArF ₄ (Ar-(<i>E</i>)-CHFCHCF ₃)	argon-(<i>E</i>)-1,3,3,3- tetrafluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₉ H ₆ O ₂ (C ₆ H ₅ C≡CCOOH)	Phenylpropionic acid	Zunwu Zhou ³ , Aaron M Pejlovas ³ , Wei Lin, Stephen G. Kukulich ³	JMS 351, 2018, 1-3
C ₅ H ₄ F ₆ O ₄ (HCOOH-(CF ₃) ₂ CHCOOH)	Formic acid-3,3,3-trifluoro-2-(trifluoromethyl)propionic acid	Javix Thomas ⁷ , Michael J. Carrillo, Agapito Serrato III, Fan Xie, Wolfgang Jaeger ⁷ , Yunjie Xu ⁷ , Wei Lin	Mol. Phys In press
C ₃ H ₂ F ₄ O ₂ (CF ₃ CFHCOOH)	2,3,3,3-tetrafluoropropionic acid	Dan A. Obenchain ¹ , Jianming Wu ⁶ , Xin Xu ⁶ , Agapito Serrato III, Will Orellana ¹ , Stephen A. Cooke ⁴ , Stewart E. Novick ¹ , Wei Lin	To be submitted
C ₃ H ₄ F ₄ O ₃ (H ₂ O-CF ₃ CFHCOOH)	Water-2,3,3,3-tetrafluoropropionic acid	Dan A. Obenchain ¹ , Jianming Wu ⁶ , Xin Xu ⁶ , Agapito Serrato III, Will Orellana ¹ , Stephen A. Cooke ⁴ , Stewart E. Novick ¹ , Wei Lin	To be submitted
C ₅ H ₈ Ne (Ne-CH ₂ =C-CCH ₂ CH ₂ CH ₂)	Neon-Methylene Cyclobutane	Andrea Minei ² , Wei Lin, Lu Kang ³ , Wallace C. Pringle ¹ , Stewart E. Novick ¹	Manuscript to be submitted
C ₄ H ₃ F ₅ O ₄ (HCOOH-CF ₃ CF ₂ COOH)	Formic acid-Pentafluoropropionic acid	Dan A. Obenchain ¹ , Stephen A. Cooke ⁴ , Stewart E. Novick ¹ , Wei Lin	Spectrum assigned
C ₃ H ₁₀ O (H ₂ O-CH ₃ CH ₂ CH ₃)	Water propane (C ¹³ isotopomers)	Dan A. Obenchain ¹ , Wei Lin, Karen Peterson ⁸ , Richard J. Saykally ⁵ , Stewart E. Novick ¹	Spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₅ H ₈ O ₂ (c- CH ₂ CH ₂ CH ₂ CHC OOH)	Cyclobutanecarboxy lic acid	Michael J. Carrillo, Shervin Fatehi, Wei Lin	Spectrum measured

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_8H_{2n+8}O_{n+3}$ ($C_8H_8O_3-(H_2O)_n$)	o-anisic acid-water complexes	Alberto Macario Susana Blanco Juan C. López	<i>PCCP in press 2019</i>
$C_7H_{2n+7}NO_{n+1}$ ($C_7H_7NO-(H_2O)_n$)	Formanilide water complexes	Pablo Pinacho Susana Blanco Juan C. López	<i>PCCP 21, 2177, 2019</i>
$C_9H_{10}O_5$ ($C_8H_8O_3-(CH_2O)_2$)	o-anisic acid – formic acid complex	Alberto Macario Susana Blanco Juan C. Lopez Yunjie Xu's Group ¹	Manuscript submitted
C_6H_7NO ($C_5H_5N-CH_2O$)	Pyridine-formaldehyde complex	Juan C. López Susana Blanco	<i>J. Phys. Chem Lett 9, 4632, 2018</i>
$C_3H_{2n+5}NO_{n+1}$ ($C_3H_5NO-(H_2O)_n$)	2-azetidinone-water complexes	Pablo Pinacho Susana Blanco Juan C. López	Spectrum observed Work in progress
$C_nH_{5n}N_nO_{2n}$ ((CH_3NO) _n -(H_2O) _n)	formamide-water complexes	Susana Blanco Juan C. López Pablo Pinacho Brooks Pate's Group ²	Spectra assigned
$C_2H_{2n+5}NO_{n+2}$ ($C_2H_5NO_2-(H_2O)_n$)	Methyl carbamate (Urethylane) water complexes	Susana Blanco Pablo Pinacho Juan C. López Z. Kisiel ³	Manuscript in prep
$C_3H_7NO_2$ $C_3H_{2n+7}NO_{n+2}$ ($C_3H_7NO_2-(H_2O)_n$)	Ethyl carbamate (Urethane) and water complexes	Pablo Pinacho Juan C. López Susana Blanco Z. Kisiel ³	Manuscript in prep

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_5H_{11}NO_2$ $C_5H_{2n+11}NO_{n+2}$ ($C_5H_{11}NO_2-(H_2O)_n$)	Butyl carbamate and water complexes	Pablo Pinacho Susana Blanco Juan C. López Z. Kisiel ³	Manuscript in prep
$C_7H_{2n+7}NO_{n+2}$ ($C_7H_7NO_2-(H_2O)_n$)	Phenyl carbamate water complexes	Pablo Pinacho Susana Blanco Juan C. López	Spectrum observed Work in progress
$C_8H_{2n+9}NO_{n+2}$ ($C_8H_9NO_2-(H_2O)_n$)	Benzyl carbamate water complexes	Pablo Pinacho Juan C. López Susana Blanco	Spectrum observed Work in progress
$C_{11}H_9N$ $C_{11}H_{2n+9}NO_n$ ($C_{11}H_9N-(H_2O)_n$)	2-Phenylpyridine and water complexes	Alberto Macario Juan C. López Susana Blanco	Manuscript in prep
$C_{2n+11}H_{6n+9}NO_n$ ($C_{11}H_9N-(ethanol)_n$)	2-Phenylpyridine ethanol complexes	Alberto Macario Juan C. López Susana Blanco	Spectra assigned Work in progress
$C_{n+11}H_{4n+9}NO_n$ ($C_{11}H_9N-(methanol)_n$)	2-Phenylpyridine methanol complexes	Alberto Macario Juan C. López Susana Blanco	Spectra assigned Work in progress
$C_{10}H_{10}O_3$ $C_{10}H_{2n+10}O_{n+3}$ ($C_{10}H_{10}O_3-(H_2O)_n$)	3-Methoxycinnamic acid and water complexes	Alberto Macario Juan C. López	Spectra observed Work in progress Susana Blanco
$C_8H_8O_3$	3-Methoxybenzoic acid (<i>m</i> -Anisic acid)	Alberto Macario Juan C. López Susana Blanco Yunjie Xu's Group ¹	Manuscript in prep
$C_9H_{10}O_5$ ($C_8H_8O_3-(CH_2O_2)$)	3-Methoxybenzoic acid (<i>m</i> -Anisic acid) formic acid complexes	Alberto Macario Juan C. López Susana Blanco Yunjie Xu's Group ¹	Spectra assigned Work in progress
$C_{15}H_{10}O_2$ $C_{15}H_{2n+10}O_{n+2}$ ($C_{15}H_{10}O_2-(H_2O)_n$)	Flavone and water complexes	Susana Blanco Juan C. López	Spectrum assigned Work in progress
$C_{15}H_{12}O_2$ $C_{15}H_{2n+12}O_{n+2}$ ($C_{15}H_{12}O_2-(H_2O)_n$)	Flavanone and water complexes	Susana Blanco Juan C. López	Spectra assigned Work in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{10}H_{2n+8}N_2O_n$ ($C_{10}H_8N_2-(H_2O)_n$)	2,2'-Bipyridine water complexes	Susana Blanco Juan C. López	Spectrum observed Work in progress
$C_9H_{12}O_2$	4-Ethylguaiacol	Susana Blanco Juan C. López Alberto Macario	Manuscript in prep
$C_8H_8O_3$ $C_8H_{2n+8}O_{n+3}$ ($C_8H_8O_3-(H_2O)_n$)	Mandelic acid and water complexes	Pablo Pinacho Susana Blanco Juan C. López	Spectrum observed
$C_8H_{10}O_2$ $C_8H_{2n+10}O_{n+2}$ ($C_8H_{10}O_2-(H_2O)_n$)	Dimethoxybenzene and water complexes	Assimo Maris ⁴ Susana Blanco Juan C. López	Spectrum observed
$C_{10}H_{16}O$ $C_{10}H_{2n+16}O_{n+1}$ ($C_{10}H_{16}O-(H_2O)_n$)	Verbenol and water complexes	Assimo Maris ⁴ Susana Blanco Juan C. López	Manuscript in prep
$C_8H_{17}NO_3$ ($C_8H_{17}NO_3$)	1-aza-12-crown-4	Juan C. López Susana Blanco	Spectrum assigned Work in progress
$C_4H_6O_3$ ($C_3H_4O_2-CH_2O$)	beta-propiolactone-formaldehyde complex	Juan C. López Susana Blanco	Spectrum assigned Work in progress
C_7H_9NO ($C_5H_5N-C_2H_4O$)	Pyridine-acetaldehyde complex	Juan C. López Susana Blanco	Manuscript in prep
$C_6H_2F_5NO$ ($C_5F_5N-CH_2O$)	Pentafluoro pyridine-formaldehyde complex	Juan C. López Susana Blanco	Spectrum assigned Work in progress
$C_8H_{11}NO$ ($C_5H_5N-C_3H_6O$)	Pyridine-acetone complex	Juan C. López Susana Blanco	Spectrum assigned
$C_9H_{13}NO$ ($C_5H_5N-C_4H_8O$)	Pyridine-2 butanone complex	Juan C. López Susana Blanco	Spectrum assigned
$C_6H_8N_2O$ ($C_5H_5N-CH_3NO$)	Pyridine-formamide complex	Susana Blanco Cristina Puzzarini ⁵ Juan C. López Lorenzo Spada ⁵	Spectrum assigned
$C_7H_{10}N_2O$ ($C_5H_5N-C_2H_5NO$)	Pyridine-N-methylformamide complex	Lorenzo Spada ⁵ Juan C. López Cristina Puzzarini ⁵ Susana Blanco	Spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_5H_{12}O$	3-methyl-butanol	Juan C. López	Spectra assigned
$C_5H_{2n+12}O_{n+1} \cdot (H_2O)_n$	water complex	Susana Blanco	Work in progress
$(C_5H_{12}O \cdot (H_2O)_n)$		Alberto Lesarri	
$C_5H_{12}ArO$	Ar complex		
$(C_5H_{12}O - Ar)$			

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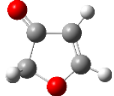
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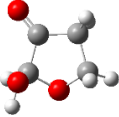
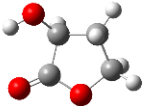
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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH ₃ N (CH ₂ NH)	Methyleneimine	Scherschligt ¹ , Douglass ¹ , Plusquellic ² , Lovas ¹	Spectrum measured near 550 GHz
CH ₅ N (CH ₃ NH ₂)	Methylamine	Scherschligt ¹ , Douglass ¹ , Plusquellic ² , Lovas ¹	Spectrum measured 530 to 600 GHz
CH ₃ NO ₂ (HCOOH-NH ₃)	Formic acid- ammonia	Grabow ³ , Lovas ¹ , Fraser ¹	Spectrum assigned For normal species
C ₂ H ₅ NO (CH ₃ OH-HCN)	Methanol-hydrogen cyanide	Lovas ¹ , Sobhanadri ⁴	Spectrum assigned for 4 isotopomers See Researchgate^a
C ₃ H ₂ O (HCCCHO)	Propynal	Plusquellic ² , Lovas ¹ , Scherschligt ¹ , Douglass ¹ ,	mm spectrum assigned
C ₃ H ₃ F ₅ O (CF ₃ CH ₂ OCHF ₂)	2,2,2-Trifluoroethyl difluoromethyl ether [RE245]	Lovas ¹ , Suenram ⁵ , Hight Walker ¹ , Dixon ^{1,6}	Lowest energy conformer, <i>anti-anti</i> , assigned.
C ₃ H ₄ O (CH ₂ =CHCHO)	Propenal	Plusquellic ² , Lovas ¹ , Scherschligt ¹ , Douglass ¹	mm spectrum assigned
C ₄ H ₄ O ₂ (_CH ₂ C(O)CH=CHO_)	3(2H)-furanone 	Lovas ¹ , Plusquellic ² , Suenram ^{1,5} , Pate ⁷ , Neill ⁸ , Muckle ⁸	Cavity & broadband spectrum assigned, manuscript in prep.

<u>FORMULA</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₆ O ₃ (_OCHOHC(O)CH ₂ C_H ₂)	Dihydro-2-hydroxy- 3(2H)-furanone 	Lovas ¹ , Plusquellic ² , Suenram ^{1,5} , Pate ⁷ , Neill ⁸ , Muckle ⁸	Cavity & broadband spectrum assigned, manuscript in prep.
C ₄ H ₆ O ₃ (_OC(O)CHOHCH ₂ C_H ₂)	Dihydro-3-hydroxy- 2(3H)-furanone 	Lovas ¹ , Plusquellic ² , Suenram ^{1,5} , Pate ⁷ , Neill ⁸ , Muckle ⁸	Cavity & broadband spectrum assigned, manuscript in prep.
C ₆ H ₁₅ O ₂ N (C ₂ H ₅ N(CH ₂ CH ₂ OH) ₂)	<i>N</i> -ethyl diethanol amine	Xu ⁹ , Liu, ⁹ Lovas ¹ , Suenram ⁵ , Fraser ¹ , Jensen ¹⁰ , Samuels ¹⁰	3 Conformers assigned
C ₁₁ H ₁₀	1-Methylnaphthalene	Plusquellic ² , Lugez ¹¹ , Hight Walker ¹ , Suenram ⁵	FTMW spectrum fit, global fit of gnd. and excited state
C ₁₁ H ₁₀	2-Methylnaphthalene	Plusquellic ² , Lugez ¹¹ , Hight Walker ¹ , Suenram ⁵	FTMW A & E state fit, of the gnd. and elec. excited state
C ₁₂ H ₁₀ O (C ₆ H ₅ -O-C ₆ H ₅)	Biphenyl ether	Onda ¹² , Schnell ¹³ , Plusquellic ² , Lovas ¹	Spectrum assigned
H ₄ OS H ₂ O-H ₂ S	Hydrogen sulfide - water dimer	Lovas ¹ , Suenram ⁵	Nine isotopic forms assigned, See Reseachgate^a
H ₄ S ₂ H ₂ S-H ₂ S	Hydrogen sulfide dimer	Das ¹⁴ , Mandal ¹⁵ , Lovas ¹ , Medcraft ¹⁶ , Walker ¹⁷ , Arunan ¹⁴	Angew. Chem. Int. Ed. 2018, 57 , 15199-15203

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₁₁ H ₁₈ O	Nopol	G. Sedo ¹ , F. E. Marshall ² , G. S. Grubbs II ²	Two Conformers Assigned Manuscript in Preparation
C ₁₀ H ₁₆ O	Myrtenol	G. Sedo ¹ , F. E. Marshall ² , G. S. Grubbs II ²	<i>J. Mol. Spectrosc.</i> 2019 , 356, 32-36.

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Formula	Name of Compound	Investigator	Present Stage of Progress
C ₃ HN	cyanoacetylene	L. Bizzocchi, ¹ M. Melosso, ² L. Dore, ² C. Degli Esposti, ² F. Tamassia, ³ H. Spahn, <i>et al.</i>	submmW and IR; ongoing; see MPE entry
CH ₂ N ₂ (H ₂ NCN)	cyanamide	A. Coutens, E. Zakharenko, H. S. P. Müller, <i>et al.</i>	¹⁵ N and ¹³ C isotopologs; <i>Astron. Astrophys.</i> 623 (2019) A93
CH ⁺	methylidyne	J. Doménech, ⁴ O. Asvany, <i>et al.</i>	<i>Astrophys. J.</i> 857 (2018) 61.
C ₂ H ₆ O ((CH ₃) ₂ O)	dimethyl ether	C. P. Endres, B. Drouin, ⁵ <i>et al.</i>	$\nu_1 + \nu_2 = 1$ ms. near subm.; higher- ν ongoing
CO	carbon monoxide	R. Gendriesch, F. Lewen, G. Klapper, H. S. P. Müller	full ms. in prep.
C ₅ H ₉ N	2-methylbutyronitrile	M. Hermanns, N. Wehres, H. S. P. Müller, <i>et al.</i>	ms on two higher lying conformers: <i>J. Mol. Spectrosc.</i> , in press; doi: 10.1016/j.jms.2018.11.009; search for excited vibrational states; one found ≤ 660 GHz; analysis ongoing
C ₂ H ₅ NO (CH ₃ C(O)NH ₂)	acetamide	V. V. Ilyushin ⁶ <i>et al.</i>	≤ 660 GHz; analysis ongoing
CH ₄ S	CH ₃ SH, CH ₃ ³⁴ SH	V. V. Ilyushin, ⁶ E. Zakharenko, L.-H. Xu, ⁷ R. M. Lees, ⁷ <i>et al.</i>	≤ 1.5 THz, $\nu_t \leq 2$; ms. on ³⁴ S isotopolog nearing completion
C ₄ H ₇ N (<i>n</i> -C ₃ H ₇ CN)	<i>n</i> -propyl cyanide	D. Liu, ⁸ A. Walters, ⁸ N. Wehres, <i>et al.</i>	several vib. states each of <i>gauche</i> and <i>anti</i> conformers; 35–506 GHz; <i>Astron. Astrophys.</i> 622 (2019) A82; ongoing
C ₂ H ₄ S	vinyl mercaptan	M.-A. Martin-Drumel <i>et al.</i>	≤ 400 GHz; <i>syn</i> and <i>anti</i> ; <i>Astron. Astrophys.</i> , in press; doi: 10.1051/0004-6361/201935032

Formula	Name of Compound	Investigator	Present Stage of Progress
CH ₂ S (H ₂ CS)	thioformaldehyde	H. S. P. Müller, A. Maeda, ⁹ <i>et al.</i>	Isotopic species: <i>Astron. Astrophys.</i> 621 (2019) A143; ≤ 1.4 THz; various vibrational states; measurements com- pleted
O ₂ S	sulfur dioxide	H. S. P. Müller	$\nu_2 = 2, \nu_1 = 1, \nu_3 = 1$; ≤ 1.5 THz; ongoing
BrF, FI	bromine and iodine mono-fluorides	H. S. P. Müller, S. Thorwirth, <i>et al.</i>	$J'' = 0, 1, \nu \leq 30$; preliminary analysis completed
C ₂ H ₃ N (CH ₃ CN)	methyl cyanide	H. S. P. Müller, B. J. Drouin, ⁵ J. C. Pearson, ⁵ <i>et al.</i>	various vibrational states and isotopic species; ongoing; inclusion of $\nu_4 = 1$ advanced.
O ₂ Ti	titanium dioxide	H. S. P. Müller, S. Brünken, <i>et al.</i>	full manuscript on 7 isotopic species in preparation
NH ₂ C ₃ H ₆ O (CH ₃ C(O)CH ₃)	amidogen acetone	H. S. P. Müller, B. J. Drouin ⁵ M. Ordu <i>et al.</i>	around 2.6 THz at JPL with one ¹³ C; ≤ 910 GHz; measurements completed for ¹³ C ₂ species, analysis of gs. nearing completion, excited states started; measurements of ¹³ C ₁ about to start
CHHeO ⁺ (He⋯HCO ⁺)	HCO ⁺ vdW complex with helium	T. Salomon, O. Asvany, <i>et al.</i>	IR & mmW/IR double reso- nance; <i>Phys. Chem. Chem.</i> <i>Phys.</i> 21 (2019) 3440
CH ₆ N ⁺ (CH ₃ NH ₃ ⁺)	protonated methyl- amine	P. Schmid <i>et al.</i>	rot.; measurements completed; manuscript in preparation
HC ₅ N	cyanodiacetylene	H. Spahn, J.-U. Grabow, ¹⁰ <i>et al.</i>	FTMW, meas. completed
CN ₂ O (N ₂ ⋯CO)	nitrogen carbon monoxide vdW complex	L. A. Surin, I. Tarabukin, ¹¹ S. Schlemmer	<i>J. Chem. Phys.</i> 148 (2018) 044313. Further assign. of "hot band" transitions to doubly excited bending mode in progress
H ₃ HeN (He⋯NH ₃)	ammonia vdW compl. with helium	L. A. Surin, S. Schlemmer, M. Hermanns	MW; search for inv. and rot.-inv. trans. of He⋯ <i>o</i> NH ₃ , He⋯ <i>p</i> NH ₃
H ₅ N (H ₂ ⋯NH ₃)	ammonia vdW compl. with hydrogen	I. Tarabukin, ¹¹ L. A. Surin, M. Hermanns, S. Schlemmer	search for rotational transi- tions of <i>p</i> H ₂ ⋯ <i>o</i> NH ₃ , <i>p</i> H ₂ ⋯ <i>p</i> NH ₃ and symmetri- cally deuterated isotopologs

Formula	Name of Compound	Investigator	Present Stage of Progress
H ₃ NNe (Ne⋯NH ₃)	ammonia vdW compl. with neon	I. Tarabukin, ¹¹ L. A. Surin, M. Hermanns, S. Schlemmer	MW; search for rot. trans. of Ne⋯pNH ₃
H ₃ N ₃ (N ₂ ⋯NH ₃)	ammonia vdW compl. with nitrogen	I. Tarabukin, ¹¹ L. A. Surin, M. Hermanns, S. Schlemmer	search for rot. transitions 12–28 GHz
CN ⁺		S. Thorwirth et al.	IR & rot.; measurements com- pleted; manuscript in prepara- tion
CH ₃ He ⁺ (He⋯CH ₃ ⁺)	CH ₃ ⁺ vdW complex with helium	M. Töpfer, O. Asvany, et al.	<i>Phys. Rev. Lett.</i> 121 (2018) 143001
C ₅ H ₉ N	3-methylbutyronitrile	N. Wehres, K. Borisov, et al.	≤ 405 GHz; ms on $v = 0$: <i>Ast- ron. Astrophys.</i> 615 (2018) A140; search for excited states ongoing; some found
CH ₄ O	CH ₃ OD	L.-H. Xu, ⁷ R. M. Lees, ⁷ et al.	≤ 1.34 THz, $v_t \leq 2$; ongoing
CH ₄ O	¹³ CH ₃ OD	L.-H. Xu, ⁷ R. M. Lees, ⁷ et al.	≤ 510 GHz, $v_t \leq 2$; ongoing
CH ₄ S	CH ₃ SD	E. Zakharenko et al.	<i>Astron. Astrophys.</i> 621 (2019) A114
CH ₄ S	¹³ CH ₃ SH	E. Zakharenko et al.	≤ 510 GHz, $v_t = 0$; analysis complete
C ₃ H ₈ O ₂	1,2-propanediol	E. Zakharenko <i>et al.</i>	further studies intended: 8th conformer, vib. exc. States
C ₃ H ₆ O	propanal	O. Zingsheim et al.	further studies ongoing
ANALYSIS/ DATABASE	Cologne Database for Molecular Spectroscopy: http://cdms.astro.uni- koeln.de/		

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C_2H_7N CH_3NHCH_3	<i>N,N</i> -Dimethyl amine	L. Nguyen, ¹ C. Gutlé ¹ W. Stahl ²	Manuscript in Preparation
$C_3H_3D_3O_2$ (CD_3COOCH_3)	Methyl acetate- D_3	L. Nguyen, ¹ I. Kleiner ¹ L.W. Sutikdja ^{2,*}	Assignments Completed
$C_3H_3D_3O_2$ (CD_3COOCH_3)	Methyl- D_3 acetate	L. Nguyen, ¹ I. Kleiner ¹ L.W. Sutikdja ^{2,*}	Experiments in Progress
C_3H_9N $C_2H_5NHCH_3$	Ethyl methyl amine	L. Nguyen ¹	Assignments Completed, Fits in Progress
$n-C_4H_5NS$ $n = 2, 4, 5$	<i>n</i> -Methylthiazol	L. Nguyen, ¹ T. Nguyen ¹ I. Kleiner ¹	$n = 2$: Manuscript in Preparation; $n = 4, 5$: Fits in Progress
C_4H_7NO $CH_3(CONH)C_2H_5$	<i>N</i> -Vinylacetamide	L. Nguyen, ¹ I. Kleiner ¹ R. Kannengießner ^{2,*}	A Species Assignments Completed, E Species in Progress
$C_4H_8O_2$ $CH_3COOC_2H_5$	Ethyl acetate	L. Nguyen ¹	<i>gauche</i> Conformer: Assignments in Progress
C_4H_8OS $CH_3(C=O)SC_2H_5$	Ethyl thioacetate	L. Nguyen, ¹ W. Stahl ² L. Tulimat ^{2,*}	Assignments in Progress
$C_4H_{11}N$ (CH_3) ₃ NH ₂	<i>tert</i> -Butyl amine	L. Nguyen ¹	Assignments Completed, Fits in Progress
C_5H_4OS	2-Thiophene- carboxaldehyde	L. Nguyen, ¹ H. Mouhib ³ R. Hariki ^{3,4}	Manuscript in Preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
n-C ₅ H ₇ N n = 1, 2, 3	n-Methylpyrrole	T. Nguyen, ¹ I. Kleiner ¹	Assignments Completed, Fits in Progress
C ₅ H ₇ NS	4,5-Dimethylthiazole	L. Nguyen, ¹ W. Stahl ² V. Van ^{2,*}	Assignments Completed, Manuscript in Preparation
C ₅ H ₇ NS	2,4-Dimethylthiazole	L. Nguyen, ¹ W. Stahl ² V. Van ^{2,*}	Assignments in Progress
C ₅ H ₈ O CH ₃ COCH=CHCH ₃	3-Penten-2-one	M. Andresen ^{1,2}	Assignments in Progress
C ₅ H ₈ O CH ₃ COC(CH ₃)=CH ₂	3-Methyl-3-Buten-2-one	M. Andresen ^{1,2}	Experiments in Progress
C ₅ H ₈ O CH ₃ COOCH ₂ CH=CH ₂	Allyl acetate	L. Nguyen ¹	Higher Energy Conformers: Assignments in Progress
C ₅ H ₈ O ₂	Coffee furanone	L. Nguyen, ¹ W. Stahl, ² V. Van ^{2,*}	Manuscript in Preparation
C ₅ H ₁₀ O CH ₃ COC ₃ H ₇	2-Pentanone	M. Andresen ^{1,2}	<i>J. Phys. Chem. A</i> 122 (2018) 7071.
C ₅ H ₁₀ O CH ₃ COCH(CH ₃) ₂	3-Methyl-2-butanone	M. Andresen ^{1,2}	Experiments in Progress
C ₅ H ₁₁ NO H(CONH)C ₄ H ₉	<i>tert</i> -Butylformamide	L. Nguyen, ¹ R. Kannengießer ^{2,*}	Manuscript in Preparation
C ₅ H ₁₃ N (CH ₃) ₃ NHCH ₃	<i>N</i> -methyl- <i>tert</i> -butyl amine	L. Nguyen ¹	Assignments Completed, Fits in Progress
C ₆ H ₆ O ₂	5-Methyl-2-furaldehyde	L. Nguyen, ¹ H. Mouhib ³ R. Hariki ^{3,4}	<i>Phys. Chem. Chem. Phys.</i> 20 (2018) 25577.
C ₆ H ₈ O	2,3-dimethylfuran	L. Nguyen, ¹ I. Kleiner ¹ H. Mouhib ⁴ R. Hariki ^{3,4}	Experiments in Progress
C ₆ H ₉ N	n,m-dimethylpyrrole n,m = 2,4; 2,5	T. Nguyen ¹ I. Kleiner ¹	Assignments Completed, Fits in Progress
C ₆ H ₁₂ O CH ₃ COC(CH ₃) ₃	Methyl <i>tert</i> -butyl ketone (pinacolone)	L. Nguyen, ¹ W. Stahl ²	Assignments Completed, Fits and Group Theory in Progress
C ₆ H ₁₂ O CH ₃ COC ₄ H ₉	2-Hexanone	M. Andresen ^{1,2}	Manuscript in Preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_6H_{12}O_2$ $CH_3(CH_2)_2COOC_2H_5$	Ethyl butyrate	L. Nguyen, ¹ L.W. Sutikdja ^{2,*}	Manuscript in Preparation
$C_6H_{12}O_2$ $C_4H_9COOCH_3$	<i>n</i> -Methyl pentanoate	M. Andresen ^{1,2}	Manuscript submitted
$C_6H_{17}NO$ $(C_2H_5)_3N \cdot H_2O$	Triethyl amine - water	L. Nguyen, ¹ R. Kannengießer ^{2,*}	Assignments in Progress
$C_7H_{14}O$ $CH_3COC_5H_{11}$	2-Heptanone	M. Andresen ^{1,2}	Manuscript in Preparation
$C_7H_{14}O_2$ $C_5H_{11}COOCH_3$	<i>n</i> -Methyl hexanoate	L. Nguyen ¹	Manuscript in Preparation
$C_7H_{10}O_4$	Dimethyl-cyclopropane-1,1-dicarboxylate	L. Nguyen, ¹ W. Stahl ² V. Van, ^{2,*} P. Groner ⁵	Manuscript in Preparation
$C_7H_{11}N$	1,2,5-Trimethylpyrrole	L. Nguyen, ¹ W. Stahl, ² V. Van ^{2,*}	Manuscript in Preparation
C_8H_9F $F(C_6H_3)(CH_3)_2$	<i>n,m</i> -Dimethylfluorbenzene <i>n,m</i> = 2,3; 2,4; 2,5; 2,6; 3,4; 3,5	L. Nguyen ¹	Assignments Completed, Fits in Progress
$C_8H_{12}S$	Tetramethylthiophene	L. Nguyen, ¹ W. Stahl, ² V. Van ^{2,*}	Assignments Completed, Fits in Progress
$C_8H_{16}O$ $CH_3COC_6H_{13}$	2-Octanone	M. Andresen ^{1,2}	Manuscript in Preparation
$C_9H_6O_2$	Coumarin	L. Nguyen, ¹ J.-U. Grabow ⁶	Manuscript in Preparation

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₃ F ₅ S [H ₂ C=CH-SF ₅]	vinylsulfur pentafluoride	W. Orellana, S. L. Stephens, W. C. Pringle, P. Groner, ^{ac} S. E. Novick, S. A. Cooke ^p	J. Chem. Phys. 149 , 144304 (2018)
C ₅ H ₄ BrN	2-bromopyridine	A. Y. Chung, E. A. Arsenault, S. L. Stephens, W. C. Pringle, C. A. Jimenez-Hoyos, S. A. Cooke, S. E. Novick	J. Mol. Spectrosc. 356 , 28-31 (2019)
C ₄ H ₁₂ [CH ₄ C ₃ H ₈]	methane propane	K. I. Peterson ^c , D. P. Pullman ^c , W. Lin, ^k A. J. Minei, ^q E. A. Arsenault, S. E. Novick	submitted, J. Phys. Chem. A
C ₃ H ₅ F ₅ S [CH ₃ CH=CH-SF ₅]	propen-1-ylsulfur pentafluoride	W. Orellana, S. L. Stephens, W. C. Pringle, S. E. Novick, S. A. Cooke ^p	manuscript in preparation
C ₄ H ₇ F ₅ S [CH ₃ CH ₂ CH=CH-SF ₅]	buten-1-ylsulfur pentafluoride	W. Orellana, S. L. Stephens, W. C. Pringle, S. E. Novick, S. A. Cooke ^p	manuscript in preparation
C ₃ H ₆ NO ₃	n-propyl nitrate	W. Orellana, S. L. Stephens, S. E. Novick, S. A. Cooke, ^p C. Brauer, ^d T. A. Blake ^d	manuscript in preparation
C ₄ H ₉ NO ₃	n-butyl nitrate	S. L. Stephens, J. A. Signore, C. Brauer, ^d T. A. Blake ^d , S. A. Cooke, ^p S. E. Novick	manuscript in preparation
C ₅ H ₁₁ I	1-iodopentane	S. L. Stephens, J. A. Signore, L. Cheng, ^{af} W. C. Bailey, ^{ag} S. A. Cooke ^p , S. E. Novick	manuscript in preparation
C ₆ H ₁₃ I	1-iodohexane	S. L. Stephens, J. A. Signore, S. A. Cooke, ^p S. E. Novick	work in progress
C ₆ H ₁₂	2-methyl-1-hexen-3-yne	S. L. Stephens, Z. Khanna, R. K. Bohn, S. E. Novick, S. A. Cooke ^p	work in progress
C ₆ H ₈ O	3-hexyne-2-one	S. L. Stephens, Z. Khanna, R. K. Bohn, S. E. Novick, S. A. Cooke ^p	work in progress
C ₈ H ₁₄ [HCC(CH ₂) ₅ CH ₃]	1-octyne	M. P. Maturo, W. Orellana, D. A. Obenchain, ^{ad} R. Melchreit, S. A. Cooke, ^p S. E. Novick	manuscript in preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₃ F ₅ O ₄ [CF ₃ CF ₂ COOH HCOOH]	perfluoropropionic acid formic acid	D. A. Obenchain, W. Lin, ^k S. E. Novick, S. A. Cooke ^p	manuscript in preparation
AgCID ₂ AgCIDH [D ₂ AgCl] [HD AgCl]	hydrogen silver chloride	D. A. Obenchain, G. S. Grubbs II, ^x D. S. Frank, H. M. Pickett, S. E. Novick	all <i>para</i> and <i>ortho</i> isotopologues assigned, manuscript in preparation
C ₃ H ₂ F ₄ O ₂ [CF ₃ CFHCOOH]	2,3,3,3-tetrafluoropropionic acid	D. A. Obenchain, ^{ad} J. Wu, ^{ac} W. Orellana, X. Xu, ^{ac} S. A. Cooke, ^p S. E. Novick, W. Lin ^k	manuscript in preparation
C ₃ H ₄ F ₄ O ₃ [CF ₃ CFHCOOH H ₂ O]	2,3,3,3-tetrafluoropropionic acid water complex	D. A. Obenchain, ^{ad} J. Wu, ^{ac} W. Orellana, X. Xu, ^{ac} S. A. Cooke, ^p S. E. Novick, W. Lin ^k	manuscript in preparation
C ₃ H ₇ F ₅ O ₅ [(H ₂ O) ₃ CF ₃ CF ₂ COOH]	pentafluoropropionic acid trihydrate	G. S. Grubbs II, ^x D. A. Obenchain, D. S. Frank, S. E. Novick, S. A. Cooke, ^p A. Serrato III, ^k W. Lin ^k	spectrum assigned
C ₆ H ₅ F ₇ O ₂ [CF ₃ CF ₂ CF ₂ COOCH ₂ CH ₃]	ethyl heptafluorobutyrate	B. E. Long, D. S. Frank, L. Hansen, D. Obenchain, R. K Bohn, ^f S. E. Novick	mostly assigned, multiple conformations, work in prog
C ₃ H ₁₀ O [H ₂ O CH ₃ CH ₂ CH ₃]	water propane (¹³ C isotopomers)	D. A. Obenchain, W. Lin, ^k K. I. Peterson, ^e R. J. Saykally, ^z W. Lin ^k	assigned
C ₈ H ₁₁ NO [NH ₂ C ₆ H ₄ CH ₂ CH ₂ OH]	4-aminophenyl ethanol	C. Bray, C. R. Rivera, E. A. Arsenault, D. A. Obenchain, S. E. Novick, J. L. Knee	assigned
C ₆ H ₅ F ₅ O ₂ [CH ₂ CHCH ₂ OOCF ₂ CF ₃]	allyl perfluoropropionate	D. S. Frank, S. E. Novick, S. A. Cooke, ^p G. S. Grubbs II	assigned
ClCuH ₂ [H ₂ CuCl]	hydrogen copper chloride	H. M. Pickett, D. A. Obenchain, G. S. Grubbs II, S. E. Novick	4 isotopologues of <i>p</i> -H ₂ CuCl and 1 isotopologue of <i>o</i> -H ₂ CuCl measured and assigned
C ₃ HF ₃ N	hexafluoroacetone imine	D. A. Obenchain, D. J. Frohman, G. S. Grubbs II, B. E. Long, W. C. Pringle, S.E. Novick, S. A. Cooke ^p	spectra assigned, manuscript in preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₅ H ₅ F ₅ O ₂ [CF ₃ CF ₂ COOCH ₂ CH ₃]	ethyl pentafluoropropionate	D. A. Obenchain, B. E. Long, B. E. Baker, R. K. Bohn ^r , S. E. Novick, S. A. Cooke ^p	work in progress, assigned
C ₅ H ₁₀ O	2-methyl-3-buten-2-ol	B. E. Long, D. A. Obenchain, S. E. Novick, S. A. Cooke ^p	work in progress, assigned
C ₅ H ₈ Ne [Ne C ₅ H ₈]	neon methylenecyclobutane	A. J. Minei, ^q W. Lin, ^k L. Kang, ⁱ W. C. Pringle, S. E. Novick	²⁰ Ne and ²² Ne isotopomers assigned
C ₄ H ₉ ArN [Ar C ₄ H ₇ NH ₂]	argon aminocyclobutane	D. J. Frohman, W. C. Pringle, S. E. Novick	work in progress
C ₅ H ₇ NNe [Ne C ₄ H ₇ CN]	neon cyanocyclobutane	D. J. Frohman, W. Ndugire, S. E. Novick, W. C. Pringle	work in progress
C ₅ H ₇ ArN [Ar C ₄ H ₇ CN]	argon cyanocyclobutane	D. J. Frohman, D. A. Obenchain, S. E. Novick, W. C. Pringle	work in progress
C ₂ F ₂ N [F ₂ CCN]	1,1-difluoro-2-nitrile-ethynyl radical	L. Kang, ⁱ S. E. Novick	manuscript in preparation
C ₄ H ₇ N	3-pyrroline; 2,5-dihydropyrrole	W. Lin, ^k D. J. Frohman, S. E. Novick	work in progress
C ₆ H ₁₀ O	3-methylcyclopentanone	A. J. Minei, ^q W. C. Pringle, S. E. Novick	work in progress
C ₆ H ₁₀ ArO [Ar C ₆ H ₁₀ O]	argon 3-methylcyclopentanone	A. J. Minei, ^q W. C. Pringle, S. E. Novick	work in progress
C ₆ H ₁₀	methylene cyclopentane	A. J. Minei, ^q W. C. Pringle, S. E. Novick	manuscript in preparation
C ₆ H ₁₀ Ar [Ar C ₆ H ₁₀]	argon methylene cyclopentane	A. J. Minei, ^q W. C. Pringle, S. E. Novick	manuscript in preparation
C ₆ H ₁₀ Ne [Ne C ₆ H ₁₀]	neon methylene cyclopentane	A. J. Minei, ^q W. C. Pringle, S. E. Novick	work in progress
C ₂ F ₆ O ₂ [CF ₃ OOCF ₃]	bis[trifluoromethoxy]peroxide	L. Kang, ⁱ S. E. Novick	spectroscopy completed
C ₄ H ₈ ArO [Ar C ₄ H ₈ O]	argon cyclobutanol	W. Lin, ^k G. Lindeke, T.T.E. Mould, W. Ndugire, S. E. Novick, W. C. Pringle	work in progress
C ₃ H ₆ S	thietane	D. McCamant, J. Schlier, S. E. Novick, W. C. Pringle	manuscript in preparation
C ₃ H ₆ ArS [Ar C ₃ H ₆ S]	argon thietane	D. McCamant, J. Schlier, S. E. Novick, W. C. Pringle	manuscript in preparation
C ₅ H ₈ Ar [Ar C ₅ H ₈]	argon cyclopentene	K. Ngogodo, L. Kang, S. E. Novick, W. C. Pringle	manuscript in preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₃ DF ₂ [F ₂ C-C≡CD]	deuterodifluororopynyl radical	L. Kang, ⁱ S. E. Novick	work in progress
C ₃ H ₁₀ Si [(CH ₃) ₃ SiH]	trimethylsilane	L. Kang, ⁱ S. E. Novick	spectroscopy completed
C ₅ H ₁₀ Si [(CH ₃) ₃ SiC≡CH]	trimethylsilylacetylene	L. Kang, ⁱ S. E. Novick	spectroscopy completed
C ₇ H ₁₀ Si [(CH ₃) ₃ SiC≡C-C≡CH]	trimethylsilyldiacetylene	L. Kang, ⁱ S. E. Novick	spectroscopy completed
CIDSi [DSiCl]	deuterated chlorosilylene	L. Kang, ⁱ S. E. Novick	work in progress
C ₃ H ₁₀ Ge [(CH ₃) ₃ GeH]	trimethyl germane	W. Lin, ^k L. Kang, ⁱ S. E. Novick	work in progress
ANALYSIS/DATABASE	Bibliography of Weakly Bound Complexes	https://wesfiles.wesleyan.edu/home/snovick/SN_webpage/vdw.pdf	updated sporadically

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CAgN (AgCN)	Silver monocyanoide	A. Nakane H. Kubota	<i>J. Mol. Struct.</i> 1164 , 539-545 (2018)
AgHO (AgOH)	Silver monohydroxide	H. Hashimoto H. Kubota	FTMW spectrum In progress
AgHS (AgSH)	Silver monohydrosulfide	H. Hashimoto H. Kubota	FTMW spectrum In progress
CAuN (AuCN)	Gold monocyanoide	H. Kubota	<i>J. Mol. Struct.</i> 1164 , 539-545 (2018)
AuHO (AuOH)	Gold monohydroxide	H. Hashimoto T. Takahashi	FTMW and mmW spectra In progress
AuHS (AuSH)	Gold monohydrosulfide	H. Kubota S. Uchida T. Takahashi	FTMW and mmW spectra In progress
AuS	Gold monosulfide	S. Mizuno	mmW spectrum Manuscript in preparation
BrNi (NiBr)	Nickel monobromide	M. Tajima	Hyperfine structure In progress
CNPd (PdCN)	Palladium monocyanoide	E. Y. Okabayashi Y. Kise	mmW spectrum In progress
CoNO	Cobalt mononitrosyl	S. Matsumoto	<i>J. Mol. Spectrosc.</i> 353 , 54-59 (2018)
ClNi (NiCl)	Nickel monochloride	E. Y. Okabayashi K. Murase	Excited electronic states In progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
ClPd (PdCl)	Palladium monochloride	Y. Kise	mmW spectrum In progress
FPd (PdF)	Palladium monochloride	Y. Kise	mmW spectrum In progress
OPd (PdO)	Palladium monoxide	T. Kurahara	mmW spectrum In progress
BrH ₂ N	Bromoamine	M. Tanaka	mmW spectrum In progress
C ₂ FI (ICCF)	Fluoroiodoacetylene ^a	Y. Shimoyama	FTMW spectrum In progress
C ₅ FN (FC ₅ N)	Fluorocyanodiacetylene	M. Hibi S. Matsumoto	FTMW spectrum In progress

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CHF ₂	Difluoromethyl radical	H. Ozeki S. Saito ¹	Analysis completed Manuscripts in preparation
N ₂ O	Nitrous oxide	H. Ozeki S. Abe	isotopologues, pressure broadening measurements
O ₃	Ozone	H. Ozeki S. Bailleux ²	main and isotopologues at 600 GHz
CH ₂ (CD ₂)	Methylene-d ₂	H. Ozeki S. Bailleux ²	THz spectrum assigned manuscript in preparation
H ₂ N (NHD)	Amidogen	K. Kobayashi ³ H. Ozeki	THz spectrum manuscript in preparation
C ₄ H ₆ N ₂ O ₂	5-Methyl Hydantoin	H. Ozeki M. Awazu K. Kobayashi ³	mmW-spectrum
INO ₂	Iodine nitrite	H. Watahiki H. Ozeki S. Bailleux ²	Spectrum assigned.
ClH	Hydrogen Chloride	H. Ozeki	Pressure broadening measurements
C ₂ H ₄ O ₂	Methyl formate	H. Ozeki K. Kobayashi ³ S. Kohjiro ⁴ K. Kikuchi ⁵	Absolute intensity measurement

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₃ H ₆ O ₂ S ((CH ₃) ₂ S...CO ₂)	Dimethyl sulfide... carbon dioxide complex	M.M. Serafin	Numerous lines observed; Stark effect experiments in progress.
C ₅ H ₁₀ O ((CH ₃) ₂ O...HCCMe)	Dimethyl ether... propyne complex	M.M. Serafin	Numerous lines observed; in progress.
C ₃ H ₇ OF ₃ ((CH ₃) ₂ O...HCF ₃)	Dimethyl ether... fluoroform complex	W. Caminati ^{a)}	Normal isotopologue assigned; dipole moment measured. Internal motion analysis.
C ₃ H ₃ F ₃ (HCCH...HCF ₃)	Acetylene...fluoroform complex	M.M. Serafin	Normal, H ¹³ CCH...HCF ₃ and DCCD...HCF ₃ spectra assigned; internal motion analysis.
C ₄ H ₁₂ Si	Diethylsilane	A.L. Steber, D.A. Obenchain, G.A. Guirgis, ^{b)} J.L. Neill, ^{c)} M.T. Muckle, ^{c)} B.H. Pate ^{c)}	²⁹ Si, ³⁰ Si and ¹³ C analysis of ((C ₂ H ₅) ₂ SiH ₂) <i>anti-anti</i> , <i>anti-gauche</i> and <i>gauche-gauche</i> conformers using CP-FTMW broadband data. Manuscript in preparation.
C ₂ HCl ₂ FOS (CHCl ₂ F...OCS)	Dichlorofluoromethane... carbonyl sulfide complex	A.L. Steber	Normal isotopologue assigned. Cl nuclear quadrupole hyperfine analysis in progress.
C ₂ HCIF ₂ OS (CHCIF ₂ ...OCS)	Chlorodifluoromethane... carbonyl sulfide complex	A.L. Steber, M.D. Foellmer	Tentative assignment made.
C ₂ HCIF ₂ O ₂ (CHCIF ₂ ...CO ₂)	Chlorodifluoromethane... carbon dioxide complex	A.L. Steber, M.D. Foellmer, J.L. Neill, ^{c)} M.T. Muckle, ^{c)} B.H. Pate ^{c)}	Tentative assignment made of broadband spectrum. Nuclear quadrupole hfs analysis in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₁₂ Ge (C ₂ H ₅) ₂ GeH ₂	Diethylgermane	A.L. Steber, G.A. Guirgis, J.L. Neill, ^{c)} M.T. Muckle, ^{c)} B.H. Pate ^{c)}	<i>Gauche-gauche</i> , <i>anti-gauche</i> and <i>anti-anti</i> conformers assigned using CP-FTMW data. ¹³ C spectra assigned for <i>gauche-gauche</i> , <i>anti-gauche</i> conformers.
C ₇ H ₃ F ₅ (C ₆ F ₅ CH ₃)	Pentafluorotoluene	A.A. Elliott, J.M. Sexton, S.A. Cooke, ^{d)} G.S. Grubbs II ^{e)}	Substitution structure and dipole moment; internal motion. Manuscript in preparation.
C ₆ ClF ₅ (C ₆ F ₅ Cl)	Chloropentafluorobenzene	A.A. Elliott, J.M. Sexton, J.L. Neill, ^{c)} M.T. Muckle, ^{c)} B.H. Pate ^{c)}	Substitution structure and nuclear hyperfine analysis; dipole moment in progress. Manuscript in preparation.
C ₄ H ₉ Br	2-bromobutane	D.A. Obenchain, Jung-Jin Oh, ^{f)} Jihyun Kim ^{f)} Heesu Jang ^{f)} Soohyun Ka ^{f)}	Three conformers assigned. ⁷⁹ Br and ⁸¹ Br nuclear quadrupole hyperfine structure. Manuscript in preparation (<i>J. Mol. Spectrosc.</i>).
C ₄ H ₇ Br	2-bromo-1-butene	Jihyun Kim, ^{f)} Jung-Jin Oh ^{f)} Heesu Jang ^{f)}	⁷⁹ Br & ⁸¹ Br isotopologues assigned.
C ₄ H ₇ Br	2-bromo-2-butene	Jihyun Kim, ^{f)} Jung-Jin Oh ^{f)} Soohyun Ka ^{f)}	⁷⁹ Br, ⁸¹ Br assigned; 2 conformers; internal rotation analysis in progress.
C ₄ H ₇ Br	4-bromo-1-butene	Jung-Jin Oh ^{f)} Heesu Jang ^{f)} Soohyun Ka ^{f)}	⁷⁹ Br, ⁸¹ Br assigned for <i>ga</i> and <i>gg</i> conformers.
C ₈ H ₁₄ O	2-ethylcyclohexanone	Jihyun Kim, ^{f)} Jung-Jin Oh ^{f)}	Normal isotopologue assigned.
C ₄ H ₈ Si (H ₂ C=CH) ₂ SiH ₂	Divinylsilane	D.A. Obenchain, G.A. Guirgis ^{b)}	Three conformers assigned; dipole moments measured. Manuscript in preparation.
C ₄ H ₆ F ₂ Si (H ₂ C=CH) ₂ SiF ₂	Difluorodivynylsilane	D.A. Obenchain, G.A. Guirgis ^{b)}	Two conformers assigned. Manuscript in preparation.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH ₃ BrF ₂ O (CHBrF ₂ ...H ₂ O)	Bromodifluoromethane... water complex	A.J. Thomas, D.A. Obenchain, A.L. Steber, ^{c)} J.L. Neill, ^{c)} B.H. Pate, ^{c)} P. Groner ^{g)}	Assigned ⁷⁹ Br, ⁸¹ Br isotopologues; all transitions doubled by H ₂ O internal rotation. Internal rotation analysis in progress.
C ₃ H ₄ F ₂ (CH ₂ F ₂ ...HCCH)	Difluoromethane... acetylene complex	D.A. Obenchain, D.L. Jurkowski, A.J. Thomas	Normal isotopologue, ¹³ C ₂ H ₂ , ¹³ CH ₂ F ₂ assigned; Dipole moment measured. Manuscript in preparation.
C ₃ H ₆ F ₂ (CH ₂ F ₂ ...C ₂ H ₄)	Difluoromethane... ethylene complex	D.A. Obenchain	Normal isotopologue assigned; internal motion analysis.
C ₃ H ₆ ClF (CH ₂ ClF...C ₂ H ₄)	Chlorofluoromethane... ethylene complex	D.A. Obenchain C.L. Christenholz	³⁵ Cl, ³⁷ Cl isotopologues assigned; internal motion analysis in progress.
C ₂ H ₂ ClFO ₂ (CH ₂ ClF...CO ₂)	Chlorofluoromethane... carbon dioxide complex	D.A. Obenchain, C.L. Christenholz	³⁵ Cl, ³⁷ Cl isotopologues assigned; internal motion analysis in progress.
C ₃ H ₄ F ₄ (CHF ₃ ...C ₂ H ₃ F)	Trifluoromethane... vinyl fluoride complex	L.F. Elmuti, S.J. Stettner, R.E. Dorris	Normal isotopologue assigned; <i>A</i> , <i>E</i> states fit in progress using XIAM and BELGI.
C ₄ H ₈ O	1,2-epoxybutane	R.E. Dorris, C.L. Christenholz	Additional measurements 6–16 GHz. ¹³ C isotopologues identified.
C ₈ H ₈ (C ₆ H ₆ ...HCCH)	Benzene...acetylene complex	E.R. Webster, R.E. Dorris, B.E. Luce	DCCD and HCCD isotopologues. Excited vibrational state analysis in progress (with McMahon, UW-Madison and Moazzen- Ahmahdi, U. Calgary).
C ₃ H ₃ BrO ₂ (C ₂ H ₃ Br...CO ₂)	Vinyl bromide...carbon dioxide complex	A.M. Anderton	⁷⁹ Br and ⁸¹ Br isotopologues assigned.
C ₂ HF ₃ Ne (C ₂ HF ₃ ...Ne)	Trifluoroethylene...neon complex	A.M. Anderton	²⁰ Ne and ²² Ne isotopologues assigned; dipole moment.
C ₂ H ₄ Cl ₂ (ClH ₂ CCH ₂ Cl)	<i>gauche</i> -1,2-dichloroethane	E.R. Webster A.S. Dikkumbura R.E. Dorris	(³⁵ Cl ₂), (³⁷ Cl ₂), (³⁵ Cl, ³⁷ Cl) species assigned; structure fit in progress.
C ₆ H ₄ F ₂ Ne	1,2-difluorobenzene... neon complex	J.M. Kang ^{h)} M.L. Grant A.G. Akmeemana S.P. Kamari	²⁰ Ne and ²² Ne isotopologue (C ₆ H ₄ F ₂ ...Ne) tentative assignments.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₄ ArF ₂ (C ₆ H ₄ F ₂ ...Ar)	1,3-difluorobenzene... argon complex	R.E. Dorris F.E. Marshall ^{e)} G.S. Grubbs II ^{e)}	Ar complex assigned; ¹³ C monomer & dimer measurements. Published <i>J. Phys. Chem. A</i> , 122 , (2018), 7385.
C ₂ H ₄ ClF	1-chloro-2-fluoroethane	A.S Dikkumbura	Normal, ³⁷ Cl, ¹³ C isotopologues assigned for <i>gauche</i> conformer; structure fit for <i>gauche</i> ; tentative assignment for <i>anti</i> conformer.
C ₈ H ₅ F (F(C ₆ H ₄)C≡CH)	3-fluorophenylacetylene	Heesu Jang ^{f)} Soohyun Ka ^{f)} Jung-Jin Oh ^{f)}	Manuscript in preparation.
C ₃ H ₄ Cl ₂	2,3-dichloropropene	A.S. Dikkumbura	Normal, ³⁷ Cl and ¹³ C isotopologues assigned for <i>gauche</i> conformer. Normal and ^{35/37} Cl species for <i>anti</i> conformer; structure fit in progress.
C ₃ F ₆	Perfluoropropene	E.N. Pinter A.L. Steber ^{d)} B. Arenas ⁱ⁾ M. Schnell ⁱ⁾	Normal and ¹³ C isotopologues assigned 5–18 GHz; dipole moment. 75–110 GHz analysis in progress. Vibrationally excited states obs.
C ₃ ArF ₆ (C ₃ F ₆ ...Ar)	Perfluoropropene...Ar complex	R.E. Dorris	Normal isotopologue assigned.
C ₃ H ₂ F ₂ O ₂ (C ₂ H ₂ F ₂ ...CO ₂)	<i>cis</i> -1,2-difluoroethene...CO ₂ complex	W.C. Trendell	Normal isotopologue assigned. Internal motion analysis in progress.
C ₄ H ₃ FO ₄	Vinyl fluoride...(CO ₂) ₂ trimer (two isomers)	P. Kannangara B.H. Pate ^{e)} C.T. West ^{e)}	Parent isotopologues for two structural forms assigned; isotopic measurements ongoing. Published <i>Chem. Phys. Lett.</i> , 706 , (2018), 538.
C ₄ H ₆ F ₂	Vinyl fluoride dimer	M.A. Martinez P. Kannangara	T-shaped form observed; normal (C ₂ H ₃ F) ₂ and ¹³ C fits; structure. Manuscript in preparation (<i>J. Mol. Spectrosc.</i>)
C ₂ H ₃ FNe C ₂ H ₃ F...Ne	Vinyl fluoride...neon dimer	P. Kannangara M.A. Martinez	²⁰ Ne fit done; consistent with an effective planar structure. Structural analysis in progress.
C ₅ H ₃ FO ₆ (C ₂ H ₃ F...(CO ₂) ₃)	Vinyl fluoride...(CO ₂) ₃ tetramer	P. Kannangara	Normal isotopologue assigned; further analysis in progress.
C ₆ H ₉ F ₃ (C ₂ H ₃ F) ₃	Vinyl fluoride trimer	P. Kannangara	Normal isotopologue assigned; further analysis in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₉ H ₁₂ F ₄ O ₂ (C ₂ H ₃ F) ₄ ...CO ₂	(Vinyl fluoride) ₄ ...CO ₂ pentamer	P. Kannangara B.H. Pate ^{c)} C.T. West ^{e)}	Spectrum assigned; work to confirm cluster composition in progress.
C ₇ H ₉ F ₃ O ₂ (C ₂ H ₃ F) ₃ ...CO ₂	(Vinyl fluoride) ₃ ...CO ₂ tetramer	P. Kannangara in progress.	Spectrum assigned; work to confirm cluster composition
C ₈ H ₉ F ₃ O ₄ (C ₂ H ₃ F) ₃ ...(CO ₂) ₂	(Vinyl fluoride) ₃ ...(CO ₂) ₂ pentamer	P. Kannangara	Spectrum assigned; work to confirm cluster composition in progress.
C ₅ H ₆ F ₂ O ₂ (C ₂ H ₃ F) ₂ ...CO ₂	(Vinyl fluoride) ₂ ...CO ₂ trimer	P. Kannangara B.H. Pate ^{c)} C.T. West ^{e)}	Spectrum assigned; work to confirm cluster composition in progress.
C ₆ H ₆ F ₂ O ₄ (C ₂ H ₃ F) ₂ ...(CO ₂) ₂	(Vinyl fluoride) ₂ ...(CO ₂) ₂ tetramer	P. Kannangara B.H. Pate ^{c)} C.T. West ^{e)}	Spectrum assigned; work to confirm cluster composition in progress.
C ₈ H ₁₂ F ₄ (C ₂ H ₃ F) ₄	Vinyl fluoride tetramer	P. Kannangara	Spectrum assigned; tentatively assigned to tetramer. Work to confirm composition ongoing.
C ₅ H ₆ F ₂ NeO ₂ (C ₂ H ₃ F) ₂ ...CO ₂ ...Ne	(Vinyl fluoride) ₂ ...Ne...CO ₂ tetramer?	P. Kannangara B.H. Pate ^{c)} C.T. West ^{e)}	Two spectra assigned (²⁰ Ne/ ²² Ne?); seems consistent with tetramer predictions; further work in progress.
C ₅ H ₂ F ₂ O ₆ C ₂ H ₂ F ₂ ...(CO ₂) ₃	1,1-difluoroethylene...(CO ₂) ₃ tetramer	T. Ariyaratne	Normal isotopologue assigned; further analysis in progress.
C ₆ H ₆ F ₆ (C ₂ H ₂ F ₂) ₃	(1,1-difluoroethylene) ₃ trimer	T. Ariyaratne	Normal isotopologue assigned; further analysis in progress.
ANALYSIS/DATABASE	Identification and assignment of cluster spectra in broadband scans using concentration dependence of intensities	P. Kannangara T. Ariyaratne B.H. Pate ^{c)} C.T. West ^{e)}	Ongoing experiments utilizing Mathcad and Python to deconvolute individual spectra. Computational tools to assist identification of cluster composition and structure.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
D ¹⁵ N	imidogen	M. Melosso ¹ , L. Dore ¹ , F. Tamassia ² , L. Bizzocchi ³ , et al.	<i>PCCP</i> 21 , 3564-3573 (2019)
H ¹⁵ N	imidogen	L. Bizzocchi ³ , M. Melosso ¹ , L. Dore ¹ , F. Tamassia ² , et al.	<i>ApJ</i> 863 , 3 (2018)
D ₂ ¹⁵ N	amidogen	M. Melosso ¹ , L. Dore ¹ , F. Tamassia ² , L. Bizzocchi ³ , et al.	<i>JQSRT</i> 222 , 186-189 (2019)
DHN	amidogen	L. Bizzocchi ³ , M. Melosso ¹ , O. Pirali ⁴ , M.A. Martin-Drumel ⁴ , et al.	THz + FIR spectrum. Manuscript in preparation
DH ¹⁵ N	amidogen	L. Bizzocchi ³ , M. Melosso ¹ , O. Pirali ⁴ , M.A. Martin-Drumel ⁴ , et al.	Measurements ongoing
DH ₂ N	ammonia-d ₁	L. Dore ¹ , C. Puzzarini ¹ , M. Melosso ¹	HFS analysis completed
D ₂ HN	ammonia-d ₂	L. Dore ¹ , C. Puzzarini ¹ , M. Melosso ¹ , Z. Kisiel ⁸	HFS analysis ongoing
D ₃ N	ammonia-d ₃	L. Dore ¹ , C. Puzzarini ¹ , M. Melosso ¹ , Z. Kisiel ⁸	HFS analysis ongoing

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_6H_{10}N_2$ (HCCCH ₂ NH ₂) ₂	propargylamine dimer	C. Degli Esposti ¹ , M. Melosso ¹ , L. Spada ^{1,7} , A. Maris ¹ , et al.	MW spectrum. Analysis completed
C_3H_7NO (HCCCH ₂ NH ₂ – H ₂ O)	propargylamine – water complex	C. Degli Esposti ¹ , M. Melosso ¹ , L. Spada ^{1,7} , A. Maris ¹ , et al.	MW spectrum. Analysis completed
C_3H_5N (HCCCH ₂ NH ₂)	propargylamine	C. Degli Esposti ¹ , L. Bizzocchi ³ , C. Puzzarini ¹ , L. Dore ¹ , et al.	<i>A&A</i> 615 , A176 (2018)
C_3H_5N (HCCCH ₂ NH ₂)	propargylamine	F. Tamassia ² , E. Canè ² , M. Melosso ¹ , C. Degli Esposti ¹ , L. Dore ¹	FIR spectrum. Analysis completed.
C_3HNO (OCCHCN)	cyanoketene	M. Melosso ¹ , L. Dore ¹ , et al.	Submm-wave spectrum. Analysis completed
$C_2H_4N_2$ (CH ₃ NHCN)	<i>N</i> -cyano-methylamine	D. Prudenzeno ³ , L. Bizzocchi ³ , M. Melosso ¹ , et al.	Measurements ongoing
C_3HN	cyanoacetylene	L. Bizzocchi ³ , F. Tamassia ² , M. Melosso ¹ , L. Dore ¹ , et al.	Higher excited states. Submm-wave and IR ongoing
C_3DN	<i>d</i> -cyanoacetylene	L. Bizzocchi ³ , F. Tamassia ² , M. Melosso ¹ , L. Dore ¹ , A. Pietropolli-Charmet ⁵ , et al.	IR / submm-wave. Manuscript in preparation
$C_2H_6O_2$ (CH ₂ OH) ₂	ethylene glycol	M. Melosso ¹ , L. Dore ¹ , et al.	THz spectrum of aGg' and gGg' conformers
C_2H_4O (CH ₂ CHOH)	vinyl alcohol	M. Melosso ¹ , L. Dore ¹ , et al.	Submm-wave spectrum (syn and anti). Manuscript submitted
C_4H_5N (c-PrCN)	cyclopropyl cyanide	M. Melosso ¹ , L. Bizzocchi ³ , A. Pietropolli-Charmet ⁵ , A. Steber ⁶ , et al.	FIR + mm-wave spectrum. Analysis ongoing

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C_2H_5N (CH_3CHNH)	ethanimine	A. Melli ¹ , M. Melosso ¹ , L. Dore ¹ , C. Puzzarini ¹ , L. Spada ^{1,2}	<i>ApJ</i> 855 , 123 (2018)
C_3H_9N (i-PrNH ₂)	isopropylamine	M. Melosso ¹ , L. Spada ⁷ , Q. Gou ⁹ , et al.	MW + submm-wave spectrum. Manuscript in preparation
C_3H_9N (n-PrNH ₂)	propylamine	M. Melosso ¹ , L. Spada ⁷ , Q. Gou ⁹ , et al.	MW + submm-wave spectrum. Manuscript in preparation
$C_3H_{11}NO$ ($C_3H_9N-H_2O$)	isopropylamine-water	C. Puzzarini ¹ , Gou ⁹ , Feng ⁹ et al.	Manuscript in preparation
$C_3H_{11}NO$ ($C_3H_9N-H_2O$)	propylamine-water	C. Puzzarini ¹ , Gou ⁹ , Feng ⁹ et al.	Manuscript in preparation
$C_4H_6S_3F_4$ ($C_2F_4S_2-C_2H_6S$)	2,2,4,4-tetrafluoro-1,3-dithiethane - dimethylsulfide complex	L. Spada ^{7,1} , D. A. Obenchain ¹⁰ , M. Juanes ¹¹ et al.	Structure Spectrum assigned
GeS	germanium sulfide	S. Thorwirth ¹² , C. Puzzarini ¹ , J. Gauss ¹³ , et al.	Sub-mmwave spectrum: manuscript in preparation
C ₂ S	thioethenylidene	C. Puzzarini ¹ , J. Gauss ¹³ , et al.	Sub-mmwave spectrum: manuscript in preparation
DHS	hydrogen sulfide-d1	C. Puzzarini ¹ , J. Gauss ¹³	hfs analysis & THz: manuscript in preparation
HSO ⁺	Hydrogen sulfur oxide cation	C. Puzzarini ¹ , V. Lattanzi ³ , S. Alessandrini ^{1,7} , J. Gauss ¹³ , et al.	Tentative assignment
CO	Carbon monoxide	C. Puzzarini ¹ , et al.	Self, N ₂ , O ₂ , H ₂ , He, Ar broadening

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ F ₃ Cl	trifluorochloro-ethylene	C. Puzzarini ¹ , L. Spada ⁷ , N. Tasinato ⁷ , P. Stoppa ⁵ , et al.	³⁵ Cl, ³⁷ Cl: Manuscript in preparation

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₅ H ₁₁ NO	Prolinol	Loru, Sanz, Pérez ² , Evagelisti ² , Pate ²	Two conf. assigned structure determined Manuscript in prep.
C ₅ H ₁₂ O ₅	Ribitol	Peña, Sanz Alonso ¹ , Alonso ¹	Chem. Eur. J. 24, 13408-13412 (2018)
C ₅ H ₁₃ NO ₂ (C ₅ H ₁₁ NO···H ₂ O)	Prolinol-H ₂ O	Loru, Sanz, Pérez ² , Evagelisti ² , Pate ²	Four conf. assigned Manuscript in prep.
C ₆ H ₁₈ O ₃	Ethanol trimer	Murugachandran, Peña, Sanz, Lamsabhi ³ , Yañez ³	Two conf. assigned
C ₆ H ₁₅ N	Triethylamine	Peña, Sanz, Myllys ⁷	Two new conf. assigned
C ₆ H ₁₇ NO	Triethylamine-H ₂ O	Peña, Sanz Myllys ⁷	One conf. assigned
C ₇ H ₇ NO ₃	Methylnitrophenol	Hussain, Burevschi, Sanz	Spectrum assigned
C ₇ H ₉ NO ₄	Methylnitrophenol-H ₂ O	Hussain, Burevschi, Sanz	Spectrum assigned
C ₇ H ₁₀ O ₂	P-cresol- H ₂ O	Hussain, Burevschi, Sanz	Spectrum assigned
C ₉ H ₁₄ O	Cyclooctanone	Burevschi, Peña, Sanz	PCCP, 21, 4331 – 4338 (2019)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_9H_{2n+14}O_{n+1}$ ($C_9H_{14}O \cdot (H_2O)_n$)	Cyclooctanone-(H_2O) _n	Burevschi, Sanz	Several hydrates assigned, manuscript in prep.
$C_{10}H_6O_2$	Naphtoquinone	Sanz, Panchagnula, Pérez ² , Evagelisti ² , Pate ²	Spectrum assigned structure determined
$C_{10}H_8O_3$ $C_{10}H_{10}O_4$ $C_{10}H_{12}O_6$	Naphtoquinone-(H_2O) ₁₋₃	Sanz, Panchagnula, Pérez ² , Evagelisti ² , Pate ²	Hydrates. assigned
$C_{10}H_{10}O$	Azulene- H_2O	Saxena, Burevschi, Sanz	Spectrum assigned
$C_{10}H_{14}O$	Carvone	Loru, Bermudez, Sanz	New conf. assigned structure determined, Manuscript in prep.
$C_{10}H_{14}O$	Perillaldehyde	Loru, Vigorito, Tang, Sanz	New conf. assigned structure determined, Manuscript in prep.
$C_{10}H_{16}$	Limonene	Santos, Loru, Sanz,	New conf. assigned structure determined Manuscript in prep.
$C_{10}H_{2n+16}O_n$ ($C_{10}H_{16} \cdot (H_2O)_n$)	Limonene-(H_2O) _n	Murugachandran, Tang, Peña, Loru, Sanz	Several hydrates and conf. assigned
$C_{10}H_{16}O$	Dihydrocarvone	Tang, Loru, Sanz,	Four conf. assigned Manuscript in prep.
$C_{10}H_{18}O$	Dihydrocarveol	Loru, Jarman, Sanz	Four conf. assigned Manuscript in prep.
$C_{10}H_8O_3$ ($C_{10}H_6O_2 \cdot \cdot H_2O$)	Perillaldehyde-(H_2O) _{1,2}	Vigorito, Loru, Sanz	Several conf. assigned
$C_{10}H_{18}O$	Geraniol	Sanz group Mohaib ⁵ , Kleiner ⁶	Spectrum observed one conf. assigned
$C_{10}H_{2n+16}O_{n+1}$ ($C_{10}H_{16}O \cdot (H_2O)_n$)	Fenchone-(H_2O) _n	Loru, Sanz Dréan ⁴ , Chrayteh ⁴	Several hydrates and conf. assigned
$C_{12}H_{22}O_2$ ($C_{10}H_{16}O \cdot \cdot CH_3CH_2OH$)	Fenchone-Ethanol	Loru, Peña, Sanz	PCCP, 21, 2938 – 2945 (2019)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{15}H_{26}O_4$	Romandolide	Burevschi, Sanz	Five conf. assigned
$C_{16}H_{22}O$ ($C_{10}H_{16}O \cdots C_6H_6$)	Fenchone-benzene	Alonso, Burevschi, Sanz	Two conf. assigned
$C_{16}H_{22}O_2$ ($C_{10}H_{16}O \cdots C_6H_5OH$)	Fenchone-phenol	Alonso, Burevschi, Sanz	One conf. assigned
$C_{17}H_{32}O_3$	Helvetolide	Burevschi, Sanz	Five conf. assigned
$C_{17}H_{30}O$	Civetone	Burevschi, Loru, Sanz	One conf. assigned
$C_{20}H_{16}$	Azulene dimer	Saxena, Burevschi, Sanz	One conf. assigned

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_2H_3F_3O_2$ ($C_2H_3F_3O-H_2O$)	2,2,2-trifluoroethanol- water	Sabrina Zinn Daniel A. Obenchain	Most assignments complete
C_3H_4N	Ethyl cyanide	Benjamin E. Arenas, Sébastien Gruet, Amanda L. Steber	Experiments Completed: Most Assignments Completed
$C_3H_4N_2$	Imidazole	Benjamin E. Arenas, Amanda L. Steber, B.M. Giuliano ¹ , L. Bizzocchi ¹	Experiments completed. Manuscripts in prep.
$C_3H_6O_2$	Methyl acetate (75- 110GHz)	Benjamin E. Arenas, Amanda L. Steber	Experiments Completed: Most Assignments Completed
$C_3H_8N_2O_4$ ($C_3H_4N_2O_2$ and $C_3H_4N_2O_2-$ (H_2O) _n n=1-2)	Hydantoin monomer and hydantoin-water complexes	Sébastien Gruet, Cristóbal Pérez	<i>PCCP</i> 20 (2018), 5545
C_3H_9NO	Alaninol	Benjamin E. Arenas, Mariyam Fatima	Experiments Completed: Most Assignments Completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C_3H_9GeI $((CH_3)_3GeI)$	Trimethyl germanium iodide	David Schmitz	Experiments Completed: Manuscript in prep.
$C_3H_{16}O_8$ $(C_3H_6O_3-(H_2O)_n \text{ n}=1-5)$	Glycolaldehyde-water complexes	Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_3H_{18}O_9$ $(C_3H_6O_3-(H_2O)_n \text{ n}=1-6)$	1,3,5-Trioxane-water complexes	Sérgio Domingos Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_5H_8O_2$ $(C_5H_8O_2-CH_3OH)$	Furan-methanol	Mariyam Fatima, Cristóbal Pérez, Daniel A. Obenchain	Experiments Completed: Manuscript in prep.
$C_5H_{10}O$	Tetrahydropyran (75-110GHz)	Sébastien Gruet	PCCP 21 (2019) 3016
$C_5H_{13}NO$	Valinol	Benjamin E. Arenas, Mariyam Fatima	Experiments Completed: Most Assignments Completed
$C_6H_{15}NO$	Leucinol	Benjamin E. Arenas, Cristóbal Pérez, Mariyam Fatima	Experiments Completed: Most Assignments Completed
$C_6H_{15}NO$	<i>iso</i> -Leucinol	Benjamin E. Arenas, Mariyam Fatima	Experiments Completed: Most Assignments Completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₇ H ₄ N ₂ O ₂	2-Nitrobenzonitrile	Jack B. Graneek	PCCP 20 (2018) 22210-22217
C ₇ H ₄ N ₂ O ₂	3-Nitrobenzonitrile	Jack B. Graneek	PCCP 20 (2018) 22210-22217
C ₇ H ₈ O	m-Cresol	Sabrina Zinn Daniel A. Obenchain	Experiments complete; assignments complete
C ₇ H ₁₂ O ₂ (C ₆ H ₈ O-CH ₃ OH)	Dimethylfuran- methanol	Mariyam Fatima, Cristóbal Pérez, Daniel A. Obenchain	Experiments Completed: Manuscript in prep.
C ₈ H ₈ O	Vinylphenylether	Mariyam Fatima, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
C ₈ H ₈ O	Styrene oxide monomer (2-8 GHz, 75-110 GHz)	Benjamin E. Arenas, Sérgio Domingos	Experiments Completed: Manuscript in prep.
C ₈ H ₁₆ O ₂	Cyclohexane-methanol	Cristóbal Pérez, Mariyam Fatima	Experiments Completed: Manuscript in prep.
C ₉ H ₁₂ O ₂ (C ₈ H ₈ O-CH ₄ O)	Vinylphenylether- methanol complexes	Mariyam Fatima, Cristóbal Pérez	<i>Beilstein J. Org. Chem.</i> 14 (2018), 1642-1654

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{10}H_{15}NO_2$	Camphor-oxime	Sérgio Domingos	Experiments Completed: Most Assignments Completed
$C_{10}H_{16}O$	Adamantanol (2–12, 75–110 GHz)	Sébastien Gruet	Experiments Completed: Most Assignments Completed
$C_{10}H_{18}O$	Linalool (2-18 GHz)	María Mar Quesada-Moreno Anna Krin	Experiments Completed: Manuscript in prep
$C_{10}H_{18}O_2$ ($C_{10}H_{16}O-H_2O$)	Thujone-water complexes	Cristóbal Pérez, Zbigniew Kisiel ²	Experiments Completed: Manuscript in prep.
$C_{10}H_{20}O$	3,7-Dimethyloct-6-en-1-ol (citronellol)	Chris Medcraft, Sérgio Domingos	Experiments Completed: Manuscript in prep.
$C_{10}H_{22}O_6$ ($C_{10}H_{20}O_5-H_2O$)	15-Crown-5-water complexes	Cristóbal Pérez, Juan Carlos Lopez ³	PCCP 21 (2019) 2875
$C_{11}H_{11}N$ ($C_6H_6-C_5H_5N$)	Benzene-pyridine complexes	Mariyam Fatima, Cristóbal Pérez, Barbara M. Giuliano ¹	Experiments Completed: Most Assignments Completed
$C_{11}H_{11}F_3O_2$ ($C_8H_8O-C_3H_3F_3O$)	Styrene oxide-3,3,3-trifluoro-1,2-epoxypropane	Sérgio Domingos Anna Krin Mark D. Marshall ⁴ Helen O. Leung ⁴	Experiments Completed: Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{11}H_{20}O_2$ ($C_{10}H_{16}O-CH_4O$)	Camphor-methanol complexes	Mariyam Fatima Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{10}H_8O$	Acenaphthenone	Donatella Loru	Experiments Completed: Most Assignments Completed
$C_{12}H_7NO_2$ $C_{12}H_9NO_3$	Naphthalimide monomer + water complex	Sérgio Domingos	Experiments Completed: Manuscript in prep.
$C_{12}H_{10}$	Acenaphthene (75-110GHz)	Sébastien Gruet, Amanda L. Steber	Experiments Completed: Manuscript in prep.
$C_{12}H_8O$	Dibenzofuran	Mariyam Fatima, Cristóbal Pérez	Experiments Completed: Most Assignments Completed
$C_{12}H_{10}O$	Diphenylether	Chris Medcraft, Sabrina Zinn Mariyam Fatima Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{12}H_{10}O_2$ ($C_{12}H_8O-(H_2O)_n$ n=1-2)	Dibenzofuran-water complexes	Mariyam Fatima Amanda L. Steber	Experiments Completed: Most Assignments Completed
$C_{12}H_{12}O_2$ ($C_{12}H_8-(H_2O)_n$ n=1-2)	Acenaphthylene-water complexes	Amanda L. Steber	Experiments Completed: Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{12}H_{16}O_4$ ($C_{12}H_{10}O-H_2O$)	Diphenylether-water ¹	Mariyam Fatima Cristóbal Pérez	<i>Angew. Chem. Int. Ed</i> 130 (2018), 9678
$C_{12}H_{16}O_4$ ($C_{12}H_{10}O-(H_2O)_n$ n=2-3)	Diphenylether-water higher-order complexes	Mariyam Fatima Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{12}H_{22}O_2$	Menthyl acetate	Anna Krin, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{12}H_{26}O_7$ ($C_{12}H_{24}O_6-H_2O$)	18-Crown-6-water complexes	Cristóbal Pérez, Juan Carlos Lopez ³	Experiments Completed: Manuscript in prep.
$C_{13}H_{12}O_2$ ($C_{12}H_8O-CH_4O$)	Dibenzofuran- methanol complexes	Mariyam Fatima, Cristóbal Pérez	Experiments Completed: Most Assignments Completed
$C_{13}H_{11}NO$ $C_{13}H_{13}NO_2$ ($C_{13}H_9N-(H_2O)_n$ n=1-2)	Phenanthridine-water complexes	Amanda L. Steber Cristóbal Pérez, Sébastien Gruet Donatella Loru	Experiments Completed: Most Assignments Completed
$C_{13}H_{12}O$ $C_{13}H_{14}O_2$ $C_{13}H_{16}O_3$ ($C_{13}H_{10}-(H_2O)_n$ n=1-3)	Fluorene-water complexes	Amanda L. Steber Sébastien Gruet	Experiments Completed: Most Assignments Completed
$C_{13}H_{12}O_2$ $C_{13}H_{14}O_3$ $C_{13}H_{16}O_4$ ($C_{13}H_{10}O-(H_2O)_n$ n=1-3)	Benzophenone-water complexes	Weixing Li Pablo Pinacho María Mar Quesada- Moreno	Experiments Completed: Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{13}H_{24}O_3$ ($C_{10}H_{16}O-C_3H_8O_2$)	Camphor-1,2-propanediol complexes	Cristóbal Pérez, Anna Krin, Mariyam Fatima	Experiments Completed: Most Assignments Completed
$C_{14}H_{12}O$ $C_{14}H_{14}O_2$ ($C_{14}H_{10}-(H_2O)_n$ n=1-2)	Phenanthrene-water complexes	Amanda L. Steber, Cristóbal Pérez Donatella Loru	Experiments Completed: Most Assignments Completed
$C_{14}H_{14}O_4$ ($C_{14}H_{12}O_3-H_2O$)	Oxybenzone-water complexes	Sérgio Domingos	<i>JPCLet</i> 9 (2018), 4963
$C_{14}H_{25}NO_2$ ($C_{14}H_{23}NO-H_2O$)	Camphor-imine + water complexes	Sérgio Domingos Pablo Pinacho	Experiments Completed: Manuscript in prep.
$C_{12}H_{22}O_2$ $C_{14}H_{28}O_3$ ($C_{10}H_{16}O-(C_2H_6O)_n$ n=1-2)	Camphor-ethanol complexes	Mariyam Fatima, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{15}H_{24}O_3$ ($C_8H_{16}O_2-C_7H_8O$)	Cyclohexane-methanol-benzyl alcohol complexes	Cristóbal Pérez, Mariyam Fatima,	Experiments Completed: Manuscript in prep.
C_8H_8O $C_{16}H_{16}O_2$ (C_8H_8O) _n n=1-2	Styrene oxide dimer	Sérgio Domingos	Experiments Completed: Manuscript in prep.
$C_{16}H_{18}O_2$ ($C_{12}H_8O-C_4H_{10}O$)	Dibenzofuran- <i>tert</i> -butylalcohol complexes	Mariyam Fatima, Cristóbal Pérez	Experiments Completed: Most Assignments Completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{16}H_{20}O$ ($C_{10}H_{14}O-C_6H_6$)	Carvone-Benzene complexes	Weixing Li María Mar Quesada- Moreno Pablo Pinacho	Experiments Completed: Most Assignments Completed
$C_{16}H_{40}O_4$ ($C_4H_{10}O$) _{n=3-4}	<i>tert</i> -butylalcohol trimer and tetramer	Cristóbal Pérez Mariyam Fatima, Pablo Pinacho	Experiments Completed: Most Assignments Completed
$C_{18}H_{11}F$	2-F-Tetrahellicene	Sérgio Domingos	Experiments Completed: Manuscript in prep.
$C_{18}H_{14}O$ ($C_{18}H_{12}-H_2O$)	Tetrahellicene-water complexes	Sérgio Domingos	Experiments Completed: Manuscript in prep.
$C_{18}H_{22}O$	4-Methylbenzylidene	Cristóbal Pérez Anna Krin	Experiments Completed: Manuscript in prep.
$C_{18}H_{24}O_2$	β -Estradiol	Sabrina Zinn	ChemPhysChem 19 (2018), 2915
$C_{20}H_{26}O$	Diadamantanyl ether	Cristóbal Pérez	Experiments Completed: Most Assignments Completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{20}H_{34}O_2$ ($C_{10}H_{16}O-C_{10}H_{18}O$)	Camphor-fenchol complexes	Mariyam Fatima, María Mar Quesada-Moreno	Experiments Completed: Most Assignments Completed
$C_{20}H_{40}O_2$ ($C_{10}H_{20}O$) ₂	Menthol dimer	Cristóbal Pérez	Experiments Completed: Most Assignments Completed
$C_{20}H_{32}O_2$ $C_{20}H_{34}O_3$ $C_{20}H_{36}O_4$ $C_{20}H_{30}O-(H_2O)_n$ n=1-3	Diadamanthyl ether-water complexes	María Mar Quesada-Moreno Pablo Pinacho	Experiments Completed: Manuscript in prep.
$C_{22}H_{26}O_2$ ($C_{12}H_{10}O-C_{10}H_{16}O$)	Diphenylether-adamantanol complex	Mariyam Fatima, Cristóbal Pérez	<i>Angew. Chem. Int. Ed.</i> 130 (2018), 9678
$C_{22}H_{36}O_2$ $C_{20}H_{30}O-C_2H_6O$	Diadamanthyl ether-EtOH complexes	María Mar Quesada-Moreno Pablo Pinacho	Experiments Completed: Manuscript in prep.
$C_{24}H_{16}O_2$ ($C_{12}H_8O$) ₂	Dibenzofuran dimer	Mariyam Fatima Amanda L. Steber, Cristóbal Pérez, Sabrina Zinn	<i>Angew. Chem. Int. Ed.</i> 131 (2019), 3140
$C_{24}H_{20}O_2$ ($C_{12}H_{10}O$) ₂	Diphenylether dimer	Mariyam Fatima, Amanda L. Steber, Cristóbal Pérez, Sabrina Zinn	<i>Angew. Chem. Int. Ed.</i> 131 (2019), 3140

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{24}H_{40}O_2$ $C_{20}H_{30}O-C_4H_{10}O$	Diadamanthyl ether- <i>tert</i> -butylalcohol complexes	María Mar Quesada- Moreno Pablo Pinacho	Experiments Completed: Manuscript in prep.
$C_{26}H_{20}$ $(C_{13}H_{10})_2$	Fluorene dimer	Mariyam Fatima Amanda L. Steber, Cristóbal Pérez, Sabrina Zinn	<i>Angew. Chem. Int. Ed.</i> 131 (2019), 3140
$C_{24}H_{22}O$ $C_{24}H_{24}O_2$ $C_{24}H_{26}O_3$ $((C_{12}H_{10})_2-(H_2O)_n \text{ n}=1-3)$	Acenaphthene dimer- water complexes	Amanda L. Steber, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{26}H_{36}O$ $C_{20}H_{30}O-C_6H_6$	Diadamanthyl ether- benzene	María Mar Quesada- Moreno Pablo Pinacho	Experiments Completed: Manuscript in prep.

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
C_3H_7ClO (ClCH ₂ CH ₂ OCH ₃)	2-chloroethyl methyl ether	Riffe, Shipman	Refining fits of excited vibrational states.
C_4H_8O (CH ₂ (O)CHCH ₂ CH ₃)	1,2-epoxybutane	Johnson, Riffe, Shipman	Refining fits of excited vibrational states.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₁₀ S CH ₃ SC ₃ H ₇	Methyl propyl sulfide	L. Tulimat, ^{1,*}	Manuscript in Preparation
C ₅ H ₆ O ₂ CH ₃ C≡CCOOCH ₃	Methyl-2-butynoate	K. Eibl ¹	Assignments Completed, Manuscript in Preparation
C ₅ H ₈ O CH ₃ C≡CCH(OH)CH ₃	3-Pentyn-2-ol	K. Eibl ¹	Assignments Completed, Manuscript in Preparation
C ₅ H ₉ O ₂ N	<i>N</i> -acetyl- <i>N</i> -methylacetamide	K. Eibl ¹ , R. Kannengießer ^{1,*} L. Nguyen ²	Manuscript in Preparation
C ₆ H ₆ O ₂	2-Acetylfuran	C. Dindic ¹	Assignments in Progress
C ₆ H ₆ OS	3-Methyl-2-thiophenecarboxaldehyde	C. Dindic ¹	Assignments in Progress
C ₆ H ₆ OS	2-Acetylthiophene	C. Dindic ¹	Assignments in Progress
C ₆ H ₈ O ₂ CH ₃ C≡CCOOCH ₂ CH ₃	Ethyl-2-butynoate	K. Eibl ¹	Assignments Completed, Manuscript in Preparation
C ₆ H ₁₀ O CH ₃ C≡CCH(OH)CH ₂ CH ₃	4-Hexyn-3-ol	K. Eibl ¹	<i>J. Chem. Phys.</i> 149 (2018) 144306
C ₆ H ₁₀ O CH ₃ COC ₄ H ₇	4-Methylpent-3-en-2-one	H. Mouhib ³	Assignments of Two Rotor Completed, 3 rd rotor in Progress
C ₆ H ₁₃ OS CH ₃ O(CH ₂) ₂ C ₃ H ₆ SH	4-Methoxy-2-methylbutane-2-thiol	H. Mouhib ³	Manuscript in Preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₇ H ₈ OS	2-Propionylthiophene	C. Dindic ¹	Assignments in Progress
C ₈ H ₁₀ O (CH ₃)C ₆ H ₄ OCH ₃	<i>m</i> -Methylanisole	L. Ferres, ¹ L. Nguyen ²	<i>J. Chem. Phys.</i> 148 , (2018) 124304
C ₈ H ₈ O ₂ CH ₃ COOC ₆ H ₅	Phenyl acetate	L. Ferres ¹	Assignments Completed, Fit in Progress
C ₈ H ₈ OS CH ₃ COSC ₆ H ₅	Phenylthioacetate	L. Ferres ¹	Assignments Completed, Fit in Progress
C ₈ H ₁₆ O CH ₂ =CHCH(OH)C ₃ H ₁₁	Octen-3-ol	H. Mouhib ³	Assignments in Progress
C ₉ H ₁₂ O (CH ₃) ₂ C ₆ H ₃ OCH ₃	2,4-Dimethylanisole	L. Ferres ¹	Under review
C ₉ H ₁₂ O	2,6-Dimethylanisole	L. Ferres ¹	Fits Completed, Manuscript in preparation
C ₉ H ₁₂ O	2,3-Dimethylanisole	L. Ferres ¹	<i>ChemPhysChem</i> 19 , (2018), 1781.
C ₉ H ₁₂ O	3,4-Dimethylanisole	L. Ferres ¹	<i>J. Phys. Chem. A</i> 123 , (2019)
C ₉ H ₁₂ O	3,5-Dimethylanisole	L. Ferres ¹	Fits Completed, Manuscript in preparation
C ₉ H ₁₂ O	2,5-Dimethylanisole	L. Ferres ¹	Assignments Completed, Fit in Progress
C ₁₀ H ₁₂ O	Rose oxide	H. Mouhib ³ V. Van ^{1,*}	Manuscript in Preparation

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₇ NO	2-aminophenol	K. Byerly G. A. Laubacher ¹ M. J. Tubergen	Spectrum recorded; assignment in progress
C ₇ H ₈ O ₂	guaiacol	A. Fox M. J. Tubergen R. M. Gurusinghe ²	Spectrum and ¹³ C isotopomers assigned, argon spectrum assigned; water complex spectra recorded; manuscript in prep.
C ₃ H ₉ NO	2-methoxyethylamine	N. Harper ³ B. Basenback ⁴ R. M. Gurusinghe ² M. J. Tubergen	¹³ C isotopomers assigned. Water complex spectrum assigned. manuscript in preparation
C ₉ H ₁₀	α-Methylstyrene, cis-β-Methylstyrene Trans-β-Methylstyrene	R. M. Gurusinghe ² M. J. Tubergen	Spectra assigned including internal Rotation. Manuscript in Preparation
C ₃ H ₆ ArO ₂	glycidol-argon	R. Wooten-Moyer ⁵ M. J. Tubergen	Spectrum assigned

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₇ H ₅ FO	2-fluorobenzaldehyde	I. Lozada, W. Sun	JPC A 122 (2018) 2060.
C ₇ H ₅ FO	3-fluorobenzaldehyde	I. Lozada, W. Sun	JPC A 122 (2018) 2060.
C ₃ HNS	isothiocyanatoethyne	W. Sun	JCP 149 (2018) 104304.
C ₅ HNS	isothiocyanato-1,3-butyne	W. Sun	JPC A 122 (2018) 7659.
C ₄ N ₂ S	cyano isothiocyanatoethyne	W. Sun	JPC A 122 (2018) 7659.
C ₇ H ₄ NO	phenyl isocyanate	W. Sun	revisions requested
C ₇ H ₅ NS	phenyl thioisocyanate	W. Sun	revisions requested
C ₈ H ₇ F	2-fluorostyrene	S. Stephens	str. analysis in progress
C ₈ H ₇ F	4-fluorostyrene	S. Stephens	str. analysis in progress
C ₃ H ₆ O ₂ S	3-mercaptopropionic acid	W. Silva	paper in preparation
C ₄ H ₈ O ₂ S	methyl 3-mercaptopropionate	W. Silva	2 conformers assigned
C ₂ H ₄ O ₂ S	thioglycolic acid	W. Silva	assignment in progress
C ₄ H ₅ NO	allyl isocyanate	O. Sogeke, W. Sun, W. Silva	paper in preparation
C ₄ H ₅ NS	allyl isothiocyanate	J. Stitsky	str. analysis in progress
C ₈ H ₇ NO	benzyl isocyanate	J. Stitsky	assignment in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₈ H ₇ NS	benzyl isothiocyanate	J. Stitsky	assignment in progress
C ₃ H ₃ S (thietane)	trimethylene sulfide	D. Desmond	MW parent, 13C, 34S, 33S- assigned far IR in progress
C ₃ H ₃ O (oxetane)	trimethylene oxide O. Mahassneh	D. Desmond 13C, 18O done	MW parent assigned far IR paper in preparation

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(Entries marked with * are collaborative studies between this laboratory and that of A. C. Legon, School of Chemistry, University of Bristol, Cantock's Close, BRISTOL BS8 1TS, UK)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH ₃ F ₃ IP*	H ₃ P...ICF ₃	S. L. Stephens	Spectrum assigned.
CH ₃ NS ₂ *	H ₃ N...CS ₂	E. Gougoula, C. Medcraft	Under peer-review (<i>J. Chem. Phys.</i>)
CH ₄ ArN ₂ O*	CH ₄ N ₂ O...Ar (urea-argon complex)	C. Medcraft	Spectrum assigned.
CH ₄ ArN ₂ S*	CH ₄ N ₂ S...Ar (thiourea-argon complex)	C. Medcraft	Spectrum assigned.
CH ₆ N ₂ OS*	CH ₄ N ₂ S...H ₂ O (thiourea-water complex)	C. Medcraft	Spectrum assigned.
C ₂ H ₂ AgI*	C ₂ H ₂ ...Ag-I	S. L. Stephens	Spectrum assigned.
C ₂ H ₂ CuF*	C ₂ H ₂ ...Cu-F	S.L. Stephens, D.P. Zaleski	Spectrum assigned, isotopic work.
C ₂ H ₂ CuI*	C ₂ H ₂ ...Cu-I	S. L. Stephens, D. Bittner	Spectrum assigned.
C ₂ H ₄ AgF*	C ₂ H ₄ ...Ag-F	S. L. Stephens	Spectrum assigned.
C ₂ H ₄ AgI*	C ₂ H ₄ ...Ag-I	S. L. Stephens	Spectrum assigned.
C ₂ H ₄ AuI*	C ₂ H ₄ ...Au-I	S. L. Stephens, M. Sprawling, D. P. Zaleski	Spectra of isotopologues assigned, manuscript in preparation.
C ₂ H ₄ CuF*	C ₂ H ₄ ...Cu-F	S. L. Stephens	Spectrum assigned.
C ₂ H ₄ CuI*	C ₂ H ₄ ...Cu-I	S. L. Stephens	Spectrum assigned.
C ₃ H ₂ F ₃ I*	C ₂ H ₂ ...ICF ₃	S. L. Stephens	Manuscript in preparation
C ₃ H ₃ N ₃ O ₂	4(5)-nitroimidazole	E. Gougoula	Spectrum assigned
C ₃ H ₉ AgNI*	(CH ₃) ₃ N...Ag-I	D. Bittner, S. L. Stephens	Spectrum assigned. Manuscript in preparation
C ₃ H ₉ F ₆ NS*	(CH ₃) ₃ N...SF ₆	D. Bittner	Spectrum assigned
C ₄ H ₃ N ₂ Br	5-bromopyrimidine	E. Gougoula	Spectrum assigned
C ₄ H ₃ N ₂ Cl	2-chloropyrimidine	E. Gougoula	Spectrum assigned
C ₄ H ₅ N ₃	2-aminopyrimidine	E. Gougoula	Spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₅ N ₃ O ₂	2-methyl-4(5)-nitroimidazole	E. Gougoula	Spectrum assigned
C ₄ H ₆ ArN ₂	1-methylimidazole-argon complex	C. Medcraft, J. Heitkämper, E. Gougoula	Spectra of isotopologues assigned
C ₄ H ₆ ArN ₂	2-methylimidazole-argon complex	E. Gougoula, C. Medcraft	Spectrum assigned.
C ₄ H ₆ ArN ₂	4-methylimidazole-argon complex	E. Gougoula, C. Medcraft	Spectrum assigned.
C ₄ H ₆ ArN ₂	5-methylimidazole-argon complex	E. Gougoula, C. Medcraft	Spectrum assigned.
C ₄ H ₆ N ₂	1-methylimidazole	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C ₄ H ₆ N ₂	2-methylimidazole	C. Medcraft, J. Heitkämper, E. Gougoula	Spectrum assigned.
C ₄ H ₆ N ₂	4-methylimidazole	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C ₄ H ₆ N ₂	5-methylimidazole	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C ₄ H ₆ N ₂ S	Thiamazole (methimazole)	E. Gougoula, C. Lacey	Spectra of isotopologues assigned.
C ₄ H ₆ ArN ₂ S	Thiamazole-argon complex	E. Gougoula, C. Lacey	Spectrum assigned
C ₄ H ₈ N ₂ O	1-methylimidazole-water complex	C. Medcraft, J. Heitkämper, E. Gougoula	Spectra of isotopologues assigned
C ₄ H ₈ N ₂ O	2-methylimidazole-water complex	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C ₄ H ₈ N ₂ O	4-methylimidazole-water complex	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C ₄ H ₈ N ₂ O	5-methylimidazole-water complex	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C ₄ H ₈ N ₂ OS	Thiamazole-water complex	E. Gougoula, C. Lacey	Spectrum assigned
C ₄ H ₈ N ₄ O*	CH ₄ N ₂ O...C ₃ H ₄ N ₂ (urea-imidazole complex)	S. Blanco (Valladolid), J.C. Mullaney, C. Medcraft,	Spectrum assigned, isotopic work.
C ₄ H ₉ NS ₂ *	N(CH ₃) ₃ ...CS ₂	E. Gougoula, C. Medcraft	Manuscript in preparation
C ₆ H ₆ N ₂ O ₂	<i>Trans</i> -urocanic acid (4-imidazoleacrylic acid)	G. Cooper, C. Medcraft, E. Gougoula	Under peer-review (<i>Phys. Chem. Chem. Phys.</i>)
C ₆ H ₈ N ₂ O ₃	<i>Trans</i> -urocanic Acid-water complex	G. Cooper, C. Medcraft, E. Gougoula	Spectrum assigned, isotopic work in progress
C ₆ H ₁₀ O ₃	Tetrahydrofuran-acetic acid complex	D.P. Zaleski, A. King	Spectrum assigned, isotopic work in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₉ N ₂ H ₈	2-phenylimidazole	E. Gougoula	Spectrum assigned
CClFPt*	FCPtCl	D. Bittner, G. Cooper, C. Medcraft	Spectra of isotopologues assigned.
CF ₂ Pt*	FCPtF	D. Bittner, G. Cooper, C. Medcraft	Spectra of isotopologues assigned.
AuBrKr	Kr...Au-Br	J. Thomas	Further isotopic species. (With M.C.L. Gerry, Vancouver).
AuH ₃ IN*	H ₃ N...Au-I	D. Bittner, S.L. Stephens	Spectrum assigned.
FIPt*	FPI	D. Bittner, G. Cooper, C. Medcraft	Spectra of isotopologues assigned.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS*</u>
C₄H₇N (<i>n</i> -C ₃ H ₇ CN)	<i>n</i> -propyl cyanide	D. Liu ¹ , A. Walters ¹ , N. Wehres ² , H. S. P. Müller ² <i>et al</i>	37–505 GHz. Ground state, and lowest vibrational states of both <i>anti</i> ($v_{30} = 1, v_{18} = 1, v_{30} = 2, v_{29} = 1, v_{18} = v_{30} = 1$) and <i>gauche</i> ($v_{30} = 1, v_{29} = 1, v_{30} = 2, v_{28} = 1, v_{29} = v_{30} = 1$) conformers A&A 622 (2019) A82 Higher vibrational states Analysis in progress
		A. Walters ¹ O. Wilkins ² H. S. P. Müller ² <i>et al</i>	

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH ₃ O ⁺ (H ₂ COH ⁺)	Protonated formaldehyde	Susanna Widicus Weaver Kevin Roenitz Luyao Zou ³ Connor Wright	Submm spectral acquisition in progress
CH ₃ O ⁺ (CH ₃ OH ₂ ⁺)	Protonated Methanol	Susanna Widicus Weaver Connor Writght Kevin Roenitz	Submm spectral acquisition in progress
CH ₅ NO (HOCH ₂ NH ₂)	aminomethanol	Susanna Widicus Weaver Hayley Bunn Brian Hays ¹ Morgan McCabe Samuel Zinga Alec Kroll	Submm spectrum acquisition and assignment in progress
EXPERIMENTAL	Microwave-Millimeterwave Double Resonance	Susanna Widicus Weaver Steven Shipman ² Kevin Roenitz Brian Hays ¹ Carson Powers Morgan McCabe Houston Smith	Published <i>J. Phys. Chem.A</i> , 2018, 122 (30), pp 6321–6327 DOI: 10.1021/acs.jpca.8b02116
EXPERIMENTAL	Submillimeter Analysis of Gas Phase Above Interstellar/Cometary Ice Analogs	Katarina Yocum Stefanie Milam ⁴ Susanna Widicus Weaver	Instrument built and initial experimental tests underway

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CHN (HCN)	hydrogen cyanide	F. Rohart ¹	lineshape analysis in progress
CHN (H ¹⁵ NC; H ¹⁵ N ¹³ C D ¹⁵ NC; D ¹⁵ N ¹³ C H ¹⁴ N ¹³ C; D ¹⁴ N ¹³ C)	hydrogen isocyanide	S. Bailleux ¹ , P. Kania ²³ , G. Wlodarczak ¹	spectrum assigned (mm+THz); manuscript in preparation
CH ₂ (CHD, CD ₂)	methylene radical	S. Bailleux ¹ , H. Ozeki ²⁴	spectrum assigned (THz); manuscript in preparation
CH ₄ O (CHD ₂ OH)	methanol	L. Coudert ⁷ , L. Margulès ¹ , R. A. Motiyenko ¹	MM+SMM+THz spectra; internal rotation analysis in progress
C ₂ HF ₃ O (HCOCF ₃)	trifluoroacetaldehyde	C. Bermudez ¹ R. A. Motiyenko ¹ L. Margulès ¹ , C. Cabezas ¹¹ J.-C. Guillemin ²	MM spectra internal rotation manuscript in preparation
C ₂ H ₃ NO ₂ (H ₃ ONCO)	methoxy-isocyanate	A. Pienkina ¹ L. Margulès ¹ , R. A. Motiyenko ¹ J.-C. Guillemin ² J. Cernicharo ⁵	MM spectra manuscript in preparation
C ₂ H ₄ O (CH ₂ DCHO)	acetaldehyde	L. Margulès ¹ , R. A. Motiyenko ¹ J.-C. Guillemin ² L. Coudert ⁷	MM+SMM spectra; internal rotation <i>A&A in press</i>

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₂ H ₅ N (CH ₃ CHNH)	ethaneimine	L. Margulès ¹ , R. A. Motiyenko ¹ J.-C. Guillemin ² B. Mc Guirre ⁹ A. Remijan ⁹	MM spectra internal rotation manuscript in preparation
C ₃ H ₂ N ₂ (NCCH ₂ CN) (NCCH ₂ NC)	malononitrile iso-cyanomethane	L. Margulès ¹ , R. A. Motiyenko ¹ J.-C. Guillemin ²	MM+SMM spectra <i>A&A in press</i> https://doi.org/10.1051/0004-6361/201834587
C ₃ H ₃ NO ₂ (CH ₃ CONCO)	acetyl-isocyanate	L. Margulès ¹ , R. A. Motiyenko ¹ J.-C. Guillemin ² I. Kleiner ⁸ V. Illyushin ³ J. Cernicharo ⁵	MM spectra internal rotation analysis in progress
C ₃ H ₄ N ₂ (CH ₃ N-CH-CN)	methylimino- acetonitrile	R. A. Motiyenko ¹ L. Margulès ¹ , J.-C. Guillemin ²	MM spectra internal rotation analysis in progress
C ₃ H ₅ N (¹³ C-CH ₃ CH ₂ CN)	ethyl cyanide	J. Pearson ¹² B. Drouin ¹² Y. ShanShan ¹² L. Margulès ¹ , R. A. Motiyenko ¹ J.-C. Guillemin ²	MM+SMM+THz spectra exc. states analysis in progress
C ₃ H ₆ O ₂ (C ₂ H ₅ COOH)	propionic acid	A. Kutsenko ³ V. Illyushin ³ R. A. Motiyenko ¹ L. Margulès ¹ , J.L. Alonso ⁶ J. Cernicharo ⁵	MM+SMM spectra; internal rotation manuscript in preparation
C ₃ H ₆ O ₃ (C ₃ H ₄ O ₂ + H ₂ O)	Methylglyoxal hydrate	S. Bteich ¹ , M. Goubet ¹ , T.R. Huet ¹	Experiments Completed Analyses in progress
C ₃ H ₇ N (CH ₃ CH ₂ CHNH)	propaneimine	L. Margulès ¹ , R. A. Motiyenko ¹ J.-C. Guillemin ² B. Mc Guirre ⁹ A. Remijan ⁹	MM+SMM spectra manuscript in preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₃ H ₇ NO (CH ₃ CH ₂ CONH ₂)	propionamide	V. Ilyushin ³ E. Alekseev ³ R. A. Motiyenko ¹ L. Margulès ¹ P. Drean ¹	MW+MM+SMM spectra; internal rotation analysis in progress
C ₅ H ₈ N ₂	2-cyanopyrrolidine	R. A. Motiyenko ¹ L. Margulès ¹ , J.-C. Guillemin ² S. Samdal ¹³	MM spectra analysis in progress
C ₇ H ₇ NO ₂	2-Nitrotoluene 3-Nitrotoluene 4-Nitrotoluene	A. Roucou ¹⁵ , I. Kleiner ⁸ , M. Goubet ¹ S. Bteich ¹ , G. Mouret ¹⁵ , F. Hindle ¹⁵ , R. Bocquet ¹⁵ , W.L. Meerts ¹⁶ , A. Cuisset ¹⁵	Experiments Completed Analyses in progress 3-NT published: <i>Chem. Phys.</i> <i>Chem. DOI:</i> 10.1002/cphc.201701266
C ₁₀ H ₈ O	1-naphthol 2-naphthol	O. Pirali ⁷ , M. Goubet ¹	Experiments Completed Analyses in progress
C ₁₀ H ₁₆ O	1-adamantanol	O. Pirali ⁷ , M. Goubet ¹ , L. Coudert ⁷	Experiments Completed Analyses in progress
C ₁₁ H ₉ N	2-phenylpyridine 3-phenylpyridine	O. Pirali ⁷ , M. Goubet ¹ , L. Coudert ⁷	Experiments Completed Analyses in progress
¹⁴ NO ⁺ ¹⁵ NO ⁺	nitrosylium ion	S. Bailleux ¹ E. Alekseev ³ J. Cernicharo ⁵	MM+SMM spectra v=0,1,2 states assigned manuscript in preparation

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₁₀ H ₁₆ O	Perillyl alcohol	F. Xie, ¹ N. Seifert M. Heger, J. Thomas	Many conformers assigned; Manuscript near completion.
C ₁₀ H ₁₈ O ₂ (C ₁₀ H ₁₆ O-H ₂ O)	Perillyl alcohol-water	F. Xie	Conformational search done; Monohydrate assignment in progress.
C ₁₀ H ₁₆ O ₆ ((C ₅ H ₈ O ₃) ₂)	Tetrahydro-2-furoic acid dimer	F. Xie ¹ N. Seifert	Several dimers assigned; Manuscripts in preparation.
C ₅ H ₁₀ O ₄ (C ₅ H ₈ O ₃ -H ₂ O)	Tetrahydro-2-furoic acid -water	F. Xie ¹ N. Seifert	Several conformers assigned; Manuscript in preparation
C ₈ H ₁₄ O ₄ (C ₅ H ₈ O ₃ -C ₃ H ₆ O)	Tetrahydro-2-furoic acid -propylene oxide dimer	F. Xie N. Seifert	Several dimers assigned; Manuscripts in preparation.
C ₇ H ₁₀ F ₆ O ₂ (C ₃ H ₂ F ₆ -C ₄ H ₈ O ₂)	1,1,1,3,3,3- hexafluoro -2-propanol (HFIP)- 1,4-dioxane	F. Xie	Spectra assigned;
C ₆ H ₁₁ F ₃ O ₃ (C ₂ F ₃ H ₃ O-C ₄ H ₈ O ₂)	2, 2, 2-trifluoroethanol (TFE)-1,4-dioxane		Assignment in progress.
C ₁₂ H ₁₅ F ₃ O ₃ (C ₈ F ₃ H ₇ O-C ₄ H ₈ O ₂)	1-phenyl-TFE (PhTFE) -1,4-dioxane		Assignment in progress.
C ₆ H ₁₆ O ₆ ((C ₃ H ₈ O ₃) ₂)	Glycerol dimer (propane-1,2,3-triol) ₂	F. Xie ¹ N. Seifert	Extensive conformational scans done; Several dimers assigned.
C ₃ H ₁₀ O ₄ C ₃ H ₁₂ O ₅ C ₃ H ₁₄ O ₆ (C ₃ H ₈ O ₃ -(H ₂ O) _{1,2,3})	Glycerol-(H ₂ O) _{1,2,3} Clusters	F. Xie J. Thomas	Extensive conformational scans done; Assignment in progress.
C ₆ H ₁₀ F ₆ O ₂ (C ₃ H ₅ F ₃ O) ₂	3,3,3-trifluoropropanol (TFP) dimer	F. Xie N. Seifert	Conformational search completed; Assignment in progress.
C ₃ H ₇ F ₃ O ₂ (C ₃ H ₅ F ₃ O-H ₂ O)	TFP-H ₂ O	F. Xie N. Seifert	Conformational search completed; Assignment in progress.
C ₈ H ₁₄ F ₆ O ₂ (C ₄ H ₇ F ₃ O) ₂	4,4,4-trifluorobutanol (TFB) dimer	F. Xie N. Seifert	Conformational search completed; Assignment in progress.
C ₄ H ₉ F ₃ O ₂ (C ₄ H ₇ F ₃ O-H ₂ O)	TFB-H ₂ O	F. Xie N. Seifert	Conformational search completed; Assignment in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₄ H ₇ NO (C ₄ H ₅ N-(H ₂ O)) C ₄ H ₉ NO ₂ (C ₄ H ₅ N-(H ₂ O) ₂)	Pyrrole-(water) _{1,2}	B. Wu ¹ J. Thomas	¹³ C of Py-1W assigned; ms in prep. Conformational search for Py-2W completed and assignment in progress.
C ₃ H ₂ F ₆ Ne (C ₃ H ₂ F ₆ -Ne)	1,1,1,3,3,3- hexafluoro -2-propanol (HFIP) -Ne	B. Wu ¹ S. Oswald N. Seifert	Spectra assigned; Manuscript in preparation.
C ₃ H ₂ ArF ₆ (C ₃ H ₂ F ₆ -Ar)	1,1,1,3,3,3- hexafluoro -2-propanol (HFIP) -Ar	B. Wu ¹ S. Oswald N. Seifert	Spectra assigned; Manuscript in preparation.
C ₃ H ₂ F ₆ N ₂ (C ₃ H ₂ F ₆ -N ₂)	HFIP-N ₂	S. Oswald ^{1,2} N. Seifert B. Wu	Spectra assigned; ¹⁴ N hfs analysis in progress; Manuscript near completion.
C ₆ H ₄ F ₁₂ C ₉ H ₆ F ₁₈ ((C ₃ H ₂ F ₆) _{2,3})	HFIP dimer and trimer	S. Oswald ^{1,2} N. Seifert	Angew. Chem. 2019. (doi.org/10.1002/anie.201813881)
C ₃ H ₄ F ₆ O (C ₃ H ₂ F ₆ -H ₂ O)	HFIP-H ₂ O	B. Wu, ¹ N. Seifert S. Oswald	A new conformer assigned. HOD, DOH and D ₂ O analysis in progress.
C ₃ H ₃ F ₅ C ₃ H ₃ F ₅ Ne (C ₃ H ₃ F ₅ -Ne)	2,2,3,3,3-pentafluoro -1-propanol (PFP) monomer and with Ne	B. Wu ¹ S. Oswald N. Seifert	One monomer fitted; Tunneling splitting observed; Detailed fits in progress
C ₆ H ₆ F ₁₀ ((C ₃ H ₃ F ₅) ₂)	PFP dimer	S. Oswald ^{1,2} B. Wu, N. Seifert	Five dimers assigned. Manuscript in preparation.
C ₃ H ₅ F ₅ O (C ₃ H ₃ F ₅ -H ₂ O)	PFP-H ₂ O	B. Wu, ¹ N. Seifert S. Oswald	Two conformers assigned. HOD, DOH and D ₂ O analysis in progress.
C ₈ H ₉ F ₃ O ₂ (C ₈ F ₃ H ₇ O-H ₂ O)	1-phenyl-2,2,2- trifluoroethanol-water	C Carlson N. Seifert	Monohydrate assigned; Manuscript near completion.
C ₁₆ H ₁₄ F ₆ O ₂ (C ₈ F ₃ H ₇ O) ₂	1-phenyl-2,2,2- Trifluoroethanol dimer	C. Carlson N. Seifert	Assignment in progress.
C ₂ F ₃ H ₆ NO (C ₂ F ₃ H ₃ O-NH ₃)	Trifluoroethanol -ammonia	C. Carlson ¹ J. Thomas, Y. Yang	Manuscript near completion.
C ₈ H ₈ O ₃	m-anisic acid (3-methoxybenzoic acid)	A. Macario Farto ³ J. Thomas	One conformer assigned; others in progress.
C ₉ H ₁₀ O ₅ (C ₈ H ₈ O ₃ -CH ₂ O ₂)	m-anisic acid-formic acid complex	A. Macario Farto ³ J. Thomas	Spectra assigned.
C ₉ H ₁₀ O ₅ (C ₈ H ₈ O ₃ -CH ₂ O ₂)	o-anisic acid (2-methoxybenzoic acid)- formic acid complex	A. Macario Farto ³ J. Thomas	Manuscript submitted.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C ₆ H ₆ F ₆ O ₂ ((C ₃ H ₃ F ₃ O) ₂)	Trifluoromethyl oxirane dimer	H. O. Leung ^{1,4} M. D. Marshall N. Seifert	Spectra assigned; manuscript in preparation.
C ₉ H ₁₈ O ₄ (C ₆ H ₁₂ O ₃ -C ₃ H ₆ O)	Solketal-propylene oxide complex	L. Evangelisti, J. Thomas C. West ⁵	Spectra assigned; manuscript in preparation.
C ₈ H ₁₂ F ₁₂ O ₄ ((C ₂ H ₃ F ₃ O) ₄)	(Trifluoroethanol) ₄	J. Thomas ¹ N. Seifert	Extensive conformational search (TFE) ₄ assignment in progress.
C ₈ H ₁₁ NO ₃ (C ₈ H ₈ O ₃ -NH ₃)	Methyl salicylate -ammonia	J. Thomas ¹	New conformers predicted; chirped and cavity assignments in progress.
C ₂ H ₇ FO ₂ C ₂ H ₉ FO ₃ C ₂ H ₁₁ FO ₄ (C ₂ H ₅ FO-(H ₂ O) ₁₋₃)	2-fluoroethanol -(water) _n	W. Huang J. Thomas	Extensive theoretical calculations for n up to 3; broadband spectra recorded; assignment in progress.
C ₄ H ₁₀ O ₅ C ₄ H ₁₂ O ₆ (C ₄ H ₆ O ₃ -(H ₂ O) ₂₋₃)	Methyl glycidate -(water) ₂₋₃	J. Thomas, Z. Wang	Theoretical calculation with n up to 3; broadband spectra recorded and assignment of others in progress.
C ₄ H ₉ NO ₃ (C ₄ H ₆ O ₃ -NH ₃)	Methyl glycidate -ammonia	J. Thomas	Broadband spectra recorded and assigned; hfs analysis with cavity measurement in progress.
C ₈ H ₁₆ O ₆ (C ₄ H ₈ O ₃ -C ₄ H ₈ O ₃)	Methyl lactate dimers	J. Thomas N. Seifert	Extensive ab initio conformational search completed; broadband spectra recorded; assignment in progress.
C ₃ H ₁₂ O ₄ C ₃ H ₁₄ O ₅ (C ₃ H ₆ O-(H ₂ O) _{3,4})	Propylene oxide -(water) _n	J. Thomas Z. Su	Extensive calculations with n=3 and 4 broadband and cavity spectra recorded; n=3 assigned and n=4 in progress.
C ₃ H ₅ FO ₂	α-Fluoropropionic acid	Y. Yang J. Thomas	New measurements and theoretical study
C ₃ H ₈ O ₂ (H ₂ O-C ₃ H ₆ O)	Acetone-water	J. Gao ¹ J. Thomas	Spectra assigned, manuscript in preparation.
CH ₆ O (CH ₄ -H ₂ O)	Methane-water	X. Liu	IR spectrum at H ₂ O v ₂ band measured; assignment in progress.
H ₃ NNe (Ne-NH ₃)	Ammonia-neon,	X. Liu	IR spectrum at NH ₃ v ₄ band assigned.
ArH ₃ N (Ar-NH ₃)	Ammonia-argon,	X. Liu	IR spectrum at NH ₃ v ₄ band assigned.
C ₃ H ₈ O ₂ (C ₃ H ₆ O-H ₂ O)	Propylene oxide -water	J. Thomas X. Liu R. Patel	Rich IR spectrum at H ₂ O v ₂ band measured; assignment in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH ₃ NO (HCONH ₂)	Formamide	F. Sunahori	High-res. IR Spectra obtained; assigned
C ₂ H ₆ N ₂ O ₂ ((HCONH ₂) ₂)	Formamide dimer	F. Sunahori	High-res. IR Spectra obtained; assignment in progress.
C ₄ H ₈ O ₃	Methyl lactate	F. Sunahori N. Borho	High-res. IR spectrum obtained; assignment in slow progress.

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Formula	Name of Compound	Name of Investigator	Present Stage of Progress
C ₂ Al	Aluminum Dicarbide	Halfen & Ziurys	<i>PCCP</i> 20 , 11047
F ₂ OS	Thionyl Fluoride	Keogh, Halfen, Ziurys	<i>J. Mol. Spec.</i> 353 , 1
OK	Potassium Oxide	Burton et al.	Manuscript in prep
BrZn 034303	Zinc Bromide	Burton & Ziurys	<i>J. Chem. Phys.</i> 150 ,
CrP 228	Chromium Phosphide	Burton, Halfen, Ziurys	<i>Chem. Phys. Lett.</i> 708 ,
BrCr	Chromium Bromide	Herman & Ziurys	Spectrum assigned

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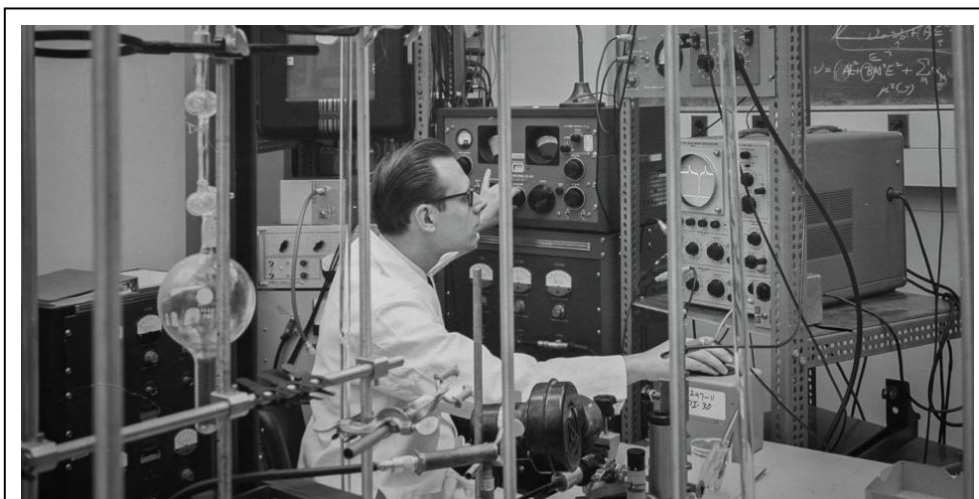
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NIST Intranet

The Loss of a NIST Treasure: Jon T. Hougen



NIST researcher Bill Kirchhoff took this photo of Jon Hougen in David Lide's microwave spectroscopy lab. Bill needed a picture of a "technician" using the equipment and Jon was the only human available. It is of course very funny, since Jon was a theoretician and not an experimentalist.

Credit: Bill Kirchhoff

By Angela R. Hight Walker

PML's Nanoscale Device Characterization Division

Jon T. Hougen, a PML scientist emeritus and longtime NIST Fellow, was born on Oct. 23, 1936, in Sheboygan, Wisconsin, and died of a sudden heart attack on Jan. 28, 2019, in Taipei, Taiwan, where he was attending a meeting of the Institute of Atomic and Molecular Sciences as a member of the institute's advisory board. He was 82 years old.



Jon Hougen

Credit: Photo courtesy of Angela Hight Walker

Jon has been a larger-than-life member of first the Bureau (NBS), then NIST, since he arrived more than 50 years ago in 1967. His brilliance was noted early in his life, leading to his leaving high school after his sophomore year to enroll at Oberlin College in 1952 on a Ford Foundation scholarship. He completed his undergraduate degree at the University of Wisconsin in 1956, then went on to earn his master's and doctoral degrees in physical chemistry at Harvard University, where he worked under the research direction of professor William Moffitt, who passed away suddenly during Jon's graduate education, and then Professor Bill Klemperer, an experimental molecular spectroscopist.

Jon's research truly changed the field of molecular spectroscopy. He was the world's leader in applying the mathematical field of group theory (https://en.wikipedia.org/wiki/Group_theory) to gas-phase spectroscopy to analyze and understand the spectral signatures of the motion, rotation and vibration of molecules.

For myself, Jerry Fraser (Sensor Science Division chief), and many other NIST scientists, the opportunity to work with Jon is the reason we came to NIST.

Jon began his career at the National Research Council (NRC) in Ottawa, Ontario, working as a postdoctoral fellow and then staff member for Gerhard Herzberg, who would go on to win the Nobel Prize (with some help from Jon — more about that later).

After nearly six years at the NRC, Jon began to feel uneasy about becoming a Canadian citizen and contemplated whether to return to the U.S. to continue his career. As luck would have it, NBS spectroscopist David Lide was delivering a set of talks at the NRC around this time.

“While at the NRC,” Lide recalls, “I was introduced to this young theoretician from Wisconsin who helped the experimental spectroscopists by devising new theoretical approaches to explain their data. On subsequent visits to Ottawa I saw that Jon’s collaboration with the senior staff was an important factor in the success of the laboratory. By this time I was chief of the NBS Infrared and Microwave Spectroscopy Section, and it was clear that a theoretician would greatly strengthen our research program. I recognized an unusual opportunity to hire a promising scientist away from what was then the world’s premier molecular spectroscopy laboratory. My division chief, Karl Kessler, concurred and agreed to find the necessary funds. Thus, Jon Hougen joined NBS in January 1967.”

Jon came in as a member of the Microwave and Infrared Spectroscopy Section, where he quickly bonded with the staff, including Art Maki, Bruce Olsen, Bill Kirchhoff and Walt Lafferty. (Sadly, Lafferty, who was Jon’s best friend, died on Dec. 27, 2018 (<https://www.legacy.com/obituaries/washingtonpost/obituary.aspx?n=walter-lafferty&pid=191119751>), a month before Jon did.) This outstanding group attracted many postdoctoral fellows and visiting scientists from the U.S. and abroad and established NBS as the place to be for molecular spectroscopy. Jon’s research interests were in quantum-mechanical and group-theoretical calculations of molecular spectroscopic constants. He studied the interactions between rotational, vibrational, and electronic motion of molecules, as well as their rotational energy levels and spectral line intensities (https://en.wikipedia.org/wiki/Spectral_line_ratios). As a theoretician, he always worked closely with experimentalists.

When Lewis Branscomb was NBS director, the Nobel Committee invited NIST’s leadership to nominate individuals to receive a Nobel Prize. In response, David Lide and Jon worked together to nominate Jon’s former supervisor, Gerhard Herzberg of the NRC. Herzberg received the Nobel Prize in chemistry in 1971 for his contributions to the knowledge of electronic structure and geometry of molecules, particularly free radicals ([https://en.wikipedia.org/wiki/Radical_\(chemistry\)](https://en.wikipedia.org/wiki/Radical_(chemistry))). While there were certainly other nominations submitted for Herzberg, Jon and David (and the strong reputation of NBS that they represented) contributed to the nomination’s success.

The numerous references to Jon’s electronic spectroscopic work in Herzberg’s classic text, *Molecular Spectra and Molecular Structure*, testifies to the major impact of Jon’s work on spectroscopy and on Herzberg’s Nobel Prize-winning research.

Hougen eventually became chief of the NBS Molecular Spectroscopy Section, a job in which he learned to detest administration and thus quickly returned to research. He was named a NIST Fellow in 1984 and served for a year as acting chief of the Molecular Physics Division. After retiring in 2001, he continued his research activities as a scientist emeritus, coming to work at NIST almost every day — including Saturdays and Sundays — up until the time of his death. Jon continued to publish at

approximately the same rate after “retirement,” even returning page proofs of an article to the *Journal of Molecular Spectroscopy* during the recent government shutdown.

MIT Professor Robert Field writes that “The 49 pages of Jon’s handbook of rotational energy-level calculations and diatomics (published as NBS 115 (<https://www.nist.gov/publications/calculation-rotational-energy-levels-and-rotational-line-intensities-diatomic-molecules>)) became the foundation of my career as a spectroscopist. Jon wrote defining guides for many areas of spectroscopy, thereby providing the foundations for many careers.”

In 2016, to commemorate Jon’s 80th birthday, NIST held a two-day symposium paying tribute to his scientific achievements, which was attended by more than 100 international experts in molecular spectroscopy. The symposium was titled “60 Years of Molecules, Motion and Matrix Elements: A Celebration of the Scientific Work of Dr. Jon T. Hougen and Colleagues,” and was video-recorded for posterity.



Jon (in the front row wearing a black suit) at the 2016 symposium celebrating his 60 years of scientific achievements. Projected onto the screen in the background is a photo of his 2001 retirement from NIST. The gatherings for both the 2001 and 2016 events included the two former NIST postdocs whom Jon went on to collaborate with on many scientific papers: Professor Li-Hong Xu of the University of New Brunswick in Canada and Isabelle Kleiner of the Laboratoire Interuniversitaire des Systèmes Atmosphériques in France.

Credit: Photo courtesy of Angela Hight Walker

Jon’s portrait has hung in the NIST “Hall of Fame” since 2003, with the following citation: “For application of quantum mechanical and group theoretical calculations to problems involving the influence of rotational, vibrational, and electronic interaction on the infrared spectra of small molecules.” He was also interviewed for an oral history (<https://cdm16009.contentdm.oclc.org/digital/collection/p16009coll2/id/7/rec/3>) by NIST’s

Standards Alumni Association. These interviews are important to understand our NIST culture.

Jon was well known for many exceptional qualities including his in-depth savant knowledge and understanding of the theory of molecular spectroscopy; his love and mastery of languages, speaking fluent Japanese, French, German and Czech (and in the process of mastering Chinese when he passed away); and his ability to communicate — his talks were infamous, standing-room-only activities at any scientific meeting he attended.

Speaking of scientific meetings, Jon attended the International Symposium on Molecular Spectroscopy annually for more than 50 years, never missing one meeting. He much preferred smaller, focused meetings — such as this symposium — where everyone who was there was really interested and engaged in the topics. Jon reached out and encouraged discussion with young scientists at these meetings. There was always a line to get to talk to him!

Jon particularly enjoyed any opportunity to work with young spectroscopists. One of the NIST postdocs that he mentored, Li-Hong Xu, went on to collaborate with Jon for decades in her role as a physics professor at Canada's University of New Brunswick, until her death three days before Jon's, on Jan. 25. Now many of Jon's NIST postdocs have postdocs of their own who Jon hosted as guest scientists at NIST. His scientific legacy will be long.

To pay tribute to Jon, an international group of researchers are now setting up a named award in his memory that will pay the travel costs for selected young spectroscopists so they can attend the International Symposium on Molecular Spectroscopy.



As shown here, Jon typically met with young scientists at every meal during each year's International Symposium on Molecular Spectroscopy.

Credit: Photo courtesy of Angela Hight Walker

Jon was a fellow of the American Physical Society, and a member of the Optical Society, the Coblenz Society, and the American Chemical Society. He served on the editorial advisory board of the *Journal of Molecular Spectroscopy* and *The Journal of Chemical Physics*. He held visiting appointments at the Institute for Molecular Science in Okazaki, Japan; Kanazawa University in Japan; Katholieke Universiteit in the Netherlands; RWTH Aachen University and the University of Hannover in Germany; and the University of Burgundy and Pierre and Marie Curie University in France.

He received numerous awards and honors for his scientific achievements, including the Coblenz Award, the NBS Gold Medal, the NBS Silver Medal, the Plyler Prize for Molecular Spectroscopy and Dynamics from the American Physical Society, the Lippincott Award from the Optical Society, and the Marcus Marci Award from the Czech Republic's Ioannes Marcus Marci Spectroscopy Society. The *Journal of Molecular Spectroscopy* dedicated a special issue to Jon in honor of his 68th birthday in 2004.

Jon was a staunch defender of good science and a formidable foe of racism and injustice. He actively supported a number of progressive causes, journalists, and candidates who were fighting for social justice. Furthermore, he quietly paid the college tuition for several students who were strongly motivated to learn, yet unable to pay their own way.

Jon also was so much fun! He loved to dance, particularly the polka, and he was very good at it.

I feel that the government shutdown probably sped Jon's death. The death of his dear friend and NIST colleague Walt Lafferty and his postdoc Li-Hong Xu during the furlough meant that Jon could not come to NIST to work though his sadness and grief. He, like me and countless other NISTers, found NIST to be a home, his colleagues to be a family, and coming to work to be a means to heal from life's troubles.

Jon is survived by his son, Torger, and daughter-in-law, Cara Neth, and by numerous nieces, nephews and cousins, whom he enjoyed visiting as often as possible. He also leaves behind his many close colleagues and friends at NIST and in the international community of spectroscopy. He was a treasure and will truly be missed.



Jon dancing the polka with me at the 2016 NIST symposium honoring him, his 80th birthday and his scientific achievements.

Credit: Photo courtesy of Angela Hight Walker

Walt Lafferty



Bill Kirchhoff Tribute

Walter J. Lafferty, * whose career at NBS/NIST spanned more than 55 years, died peacefully on December 27, 2018. He was 84. After receiving a B.S. with honors in chemistry from the University of Delaware (1956) he earned his Ph.D. in physical chemistry from MIT (1960). His thesis, under the direction of Professor R.C. Lord, was on the far infrared spectrum of trimethylene oxide and trimethylene oxide-d6.

After serving a post-doctoral year in the chemistry department at Johns Hopkins University, Walt joined NBS on January 2, 1962 as a research chemist in the Physics Division's Radiometry Section headed by Earle Plyler. On his retirement in 1995 he became a Scientist Emeritus in the Sensor Science Division of PML—a position he held for the next 22 years until he stepped down in 2017.

His measurements and compilations helped accelerate the growth of computational chemistry by providing the critical molecular data to facilitate the development, optimization, and validation of the models and algorithms. His successes in this area included the first correct determination of the structures of diborane (B_2H_6) and carbon suboxide (OCCCO) which provided significant challenges to electronic structure theoreticians because of the exotic bonding they exhibit. His measurements of the infrared and near-infrared discrete and continuum spectra of molecules important in planetary atmospheres, such as HOCl, NO_2 , B_2H_6 , $ClNO_3$, H_2O , O_2 , N_2 , SO_2 , and ClO_2 were a major contribution, providing data for modeling atmospheric radiative transfer, determining atmospheric transmittance, and extracting atmospheric gas concentration profiles through remote sensing. He also made seminal contributions to the structure and dynamics of the hydrogen bond through his successful analysis of the infrared spectra of the highly nonrigid hydrogen fluoride dimer—the prototypical hydrogen-bonded system. Walt's expertise in the analysis of such complex spectra was unsurpassed, leading to numerous requests from outside scientists for help on their spectroscopy problems.

Walt published over 140 technical papers and received a *Silver Medal Award* in 1975. His many other honors included visiting *Leverhulm Fellow*, University of Reading, England (1971–1972); visiting professor, Univ. de Pierre et Marie Curie, Paris (four times); visiting professor, Univ. de Paris Sud (eleven times); and *Iberdrola Visiting Professor* in the Molecular Physics Department

in the Institute of the Structure of Matter of CSIC (Spanish National Research Council) in Madrid (1997). He was a member of the Coblentz Society, American Physical Society, and the American Chemical Society.

The May 2005 *Journal of Molecular Structure* was dedicated to him. The issue, “[Molecular Spectroscopy and Structure](#) - A Collection of Invited Papers in Honor of Dr. Walter J. Lafferty.” includes a two-page biographical sketch of Walt written by James R. Durig.¹

In 2014 Walt was inducted into the NIST Portrait Gallery for his “seminal contributions to measurement and compilation of spectral, structural, and force-field molecular properties important in predictive chemical and physical modeling.”

Walter J. Lafferty was born February 10, 1934 in Wilmington, Delaware and was educated in the Delaware public schools. He met his wife, Mary, at a 1957 New Year’s Party and they were married in June 1959. His hobbies included amateur radio and bridge.

He is survived by his wife, Mary (Patten) Lafferty; his daughters, Anne Lafferty, Maura Lafferty, Clare Lafferty, Ellen Lafferty, Paula Lafferty, and Brenda Kawahara; his sister, Margaret Lazusky; and four grandchildren.

Sources: *The Washington Post*, Dec. 30, 2018; *Journal of Molecular Structure*, May 2005; and *SAA Newsletter* archives.

Note from Wallace “Pete” Pringle

Walter J. Lafferty of Silver Spring MD passed away on December 27, 2018. Walt entered MIT to earn a PhD under the direction of Richard C. Lord following his undergraduate studies at University of Delaware. He was a pioneer of far infrared spectroscopy, helping to develop the first vacuum FIR spectrometers. After a postdoctoral fellowship at Johns Hopkins, he joined the National Bureau of Standards in Washington, DC. At NBS that became NIST in Gaithersburg MD, he published over 100 papers and a book. He had strong collaborations in France, England and Spain specializing in high resolution infrared spectroscopy. Walt also contributed to microwave spectroscopy. He is survived by his wife, Mary, six daughters and four grandchildren.

Washington Post obituary

WALTER J. LAFFERTY

Of Silver Spring, MD, died peacefully on December 27, 2018. After receiving an undergraduate degree in chemistry at the University of Delaware, he entered M.I.T. and earned a Ph.D. in physical chemistry. He then served a post-doctoral year in the chemistry department at Johns Hopkins University. After starting his long career at the National Bureau of Standards (NBS),

¹ The biography, as well as all of the articles published in the collection, can be read at <https://www.sciencedirect.com/journal/journal-of-molecular-structure/vol/742/issue/1>.

now known as the National Institute of Standards and Technology (NIST), he co-authored over 100 papers as well as a book. He was awarded the Leverhulme Fellowship, allowing him to spend a year teaching and doing research at Reading University in the U.K., and a Silver Medal for Meritorious Service from the Department of Commerce. After retiring from NIST in 1997, he went to Madrid for six months to lecture and do research at the Spanish National Research Council. Despite retiring he continued working as an emeritus at NIST until recently. His portrait is now a permanent part of the NIST "Gallery of Alumni." His hobbies included amateur radio and bridge. Surviving Walter are his wife, Mary (Patten) Lafferty; his daughters, Anne Lafferty, Maura Lafferty, Clare Lafferty, Ellen Lafferty, Paula Lafferty, and Brenda Kawahara; his sister, Margaret Lazusky; and four grandchildren, Megan, Lauren and Patrick Kawahara, and Justin Baba. Visitation will begin at 11 a.m. on Wednesday, January 2, 2019 at Our Lady of Grace Catholic Church, 15663 Norbeck Blvd, Silver Spring, MD 20906, where Mass of Christian Burial will take place at 12 noon. Interment to follow at Gate of Heaven Cemetery, Silver Spring, MD. In lieu of flowers, donations may be made to NAMI (National Alliance for the Mentally Ill), P.O. Box 49104, Baltimore, MD 21297. Arrangements by Cole Funeral Services, P.A., Rockville, MD.

www.colefuneral.com

Li-Hong Xu



Tribute from Yunjie Xu

Li-Hong leaves behind an extraordinary record of involvement and accomplishment in an incredibly wide range of activities. Her professional life as a physicist took her all around the world to conferences and research laboratories, and she was highly respected by the international community. She is remembered as a dynamic and engaging speaker, and gave many invited seminars and panel presentations. Her research activities focused on applying high resolution eigenstate resolved spectra both at room temperature and in a jet-cooled molecular-beam to probe intramolecular Vibrational energy Relaxation promoted by rapid methyl-top internal rotation and modeling of the large-amplitude torsional motion in methanol and its interaction with small amplitude vibrations, as well as laboratory-based astrophysics. Li-Hong had great skill at managing and making connections, and her lab was a lively place. She attracted post-doctoral fellows and visiting researchers and students from Belgium, France, Russia, Iran, the Czech Republic, China and the US, and had a large number of undergraduate summer and work-study students over the years, giving them a good start on their careers.

Li-Hong had a special interest in promoting women in science, and served for 3 years as the Chair of CEWIP, the Committee to Encourage Women in Physics, a division of the Canadian Association of Physicists for which she arranged speakers and special sessions at our annual meetings. She was a member of the Canadian delegation to ICWIP, the big International Conferences on Women in Physics held in South Korea and South Africa, and was closely involved with the 2014 ICWIP meeting here in Canada where she was the lead author of the paper, "Women in physics in Canada". Locally, she organized special optics workshops for girls at the Public Library uptown, gave talks and demonstrations at local schools, and always set up tables at the UNBSJ open houses and special events where she recruited her girl students to show off fun experiments to encourage and stimulate people's interest in physics and promote UNB.

In addition to all her research and outreach work, of course, Li-Hong was also busy teaching, and again she displayed great enthusiasm and innovative approaches. In her first-year course, she introduced the idea of "Party Physics" where in each lecture she would have a party trick, a special demonstration or short online video to interest and sometimes amaze her students. Often the students would come up with their own ideas for the party piece, which made it a lot of fun for everyone. This was recognized in 2014 with one of the Inaugural prizes in the "Change One Thing" challenge by the UNB Centre for Enhanced Teaching & Learning. As well as her formal teaching, an important legacy left by Li-Hong was the

training and inspiration she gave to the 32 undergraduate students who worked in her lab as research assistants over the years, representing a strong and lasting contribution to the future community.

The third pillar of a university career is service to the institution and the academic community, and here as well Li-Hong has left a memorable mark. She was Acting Department Chair for several years, and served multiple terms on many faculty and University committees. She became Director of the Music Program of the Lorenzo Society 7 years ago, and will be remembered for her warm introductions (and also her welcoming bowl of chocolates) at the Saint John String Quartet noon-hour concerts. She organized a number of student-led concerts, and arranged for UNB students and staff to join forces with the DalMedNB medical students in the Heartbeat Choir and the Ceol Ceilidh band, greatly enriching the cultural life at the university. She was an active member of the AUNBT, the faculty union, and took her turns on the picket line at the university gates in that cold January of 2014 during the short faculty strike. Nationally, she became the “go-to person” from the physics community for the Natural Sciences and Engineering Research Council in Canada, and served on the International Advisory Committees for conferences and journals. Now Li-Hong was never boastful about her achievements, but she was certainly very proud of them and one wall of her office is filled with Certificates of Appreciation and Awards from UNB, the NSERC Research Council, the US National Institute of Standards and Technology, the Canadian Space Agency, and other institutions all recognizing her contributions.

Note from Jens-Uwe Grabow

Many of us might know Li-Hong as a quite private but even more so as a very warm person. She always cared about the people working with her or around her. During her time at the US National Institute of Standards and Technology, she was – despite being very devoted to her research and constantly imposing long working hours on herself – frequently inviting her NIST colleagues to her home in the evening. Pure leisure, like spending the evening at a bar, was not that meaningful for her, but cooking for friends was and she enjoyed it very much. She liked to say “I am not you mother, you know!” but, in fact, she said this only after pointing out a ‘deficit’ that she had identified followed by some advice how to fix it. Occasionally, Li-Hong was worried: Worried about the well-being of others, maybe more than about her own. Like a mother – which she refused admit, while laughing though – would care and help.

Tribute from Shui-Ming Hu

Li-Hong was born in late 1950’s in a small town a hundred miles away from Shanghai. Similar to many other Chinese born in the same era, Li-Hong grew up experiencing the some of the most dramatic changes happening in China. As the 2nd girl in her family, Li-Hong was not a favorite in her grandmother’s eye, but she was loved and protected by her parents. Growing up during the Cultural Revolution, she did not have the opportunity to take regular classes in school. As a result, she kept enthusiasm for learning in her whole life. Upon her graduation from high school, following the policy applied by the government, Li-Hong should be sent for “re-education” in a remote farm together with her classmates. Her parents, however, attempted firmly to prevent from happening and protected her to remain at home. In order to avoid detection, Li-Hong had to frequently move residencies. Four such years did Li-Hong live in the shadows before her parent’s wisdom turned to effect when Deng Xiaoping reinstated the formal university entrance exam system in 1977. With borrowed textbooks and self-study during those hot summer months, Li-Hong was among a small elite group who got into university, though once again she had to obey her parents’ wishes to stay close to her hometown. In the Suchow University, she had a lot to learn and was longing for knowledge. Graduating with highest honors, Li-Hong was appointed to remain in her alma mater as an assistant professor, and stayed there until her leave for Canada in the late 1980’s.

Dr. Xu regards New Brunswick as her second home after China, and she also devoted considerable energy to the Chinese community and the Asian Heritage Society of New Brunswick. When China became more open to the world, she paid more efforts to bridge the communication between Chinese and North American spectroscopists. Her enthusiasm affected people around her when she was discussing about setting a new series of spectroscopy conferences in Asia. The idea soon became true and the first two of such conferences were held in Japan and Taiwan. Li-Hong had been keenly looking forward to the 3rd meeting coming up in March of 2019 in Hefei, China. She also expressed her desire to transfer her knowledge and experience in molecular spectroscopy to young students, for which she formally accepted the assignment to teach a 40-hours course in the summer of 2018 at University of Science and Technology of China. Unfortunately, just a few weeks before her trip, she was diagnosed with cancer. Although she could not contribute more to the community she loved so much, her passion impressed all the people around her.