

**MICROWAVE SPECTROSCOPY INFORMATION LETTER**

**VOL. LXIII**

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## 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](http://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](mailto: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**.

*Due to the COVID-19 pandemic, this edition has been delayed from its usual dissemination date and was not printed. This is the first time in the history of the Letter that all distributed copies were in electronic format.*

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**In Memoriam**

James R. Durig

(Written by Peter Groner, Victor F. Kalasinsky, Y. S. Li, and Charles J. Wurrey; Obituary provided by Gamil Guirgis)

After Index

Harald Møllendal

(Written by Peter Kleebe, Svein Samdal, and Einar Uggerud; Picture from Alberto Lesarri)

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>2</sub> H <sub>3</sub> NO	Methyl isocyanate <sup>a,b,d</sup>		ApJ Sup.Ser 245,2 (2019)
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Vinyl Alcohol		mmw-sub wave spectrum
C <sub>2</sub> H <sub>3</sub> NO	Propynal		submitted
C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	Glycolamide		A&A 2020
C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	Acetohydroxamic		ms. In preparation
C <sub>3</sub> H <sub>3</sub> NO	Propiolamide <sup>d</sup>		ms. In preparation
C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub>	Cyanoacetic acid		spectrum assigned
C <sub>3</sub> H <sub>4</sub> O <sub>4</sub>	Malonic Acid		LA-CPFT spectrum
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O	Cyanoacetamide		LA-MB-FTMW
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	Lactaldehyde		ms. in preparation
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	Cycloserine <sup>e,f</sup>		LA-CPFT spectrum
C <sub>3</sub> H <sub>7</sub> N <sub>3</sub> O <sub>2</sub>	Glycociamine		LA-MB-FTMW
C <sub>4</sub> H <sub>2</sub> O <sub>4</sub>	Squaric acid		Chem. Eur.J. 2019, 25,10748
C <sub>4</sub> H <sub>4</sub> O <sub>6</sub>	Malic acid		ms. In preparation
C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>	Tartaric Acid		ms. in preparation
C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O	Creatinine <sup>e,f</sup>		ms. in preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O <sub>3</sub>	Cytosine-water		ms. in preparation
C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> S	Homocysteine		ms. in preparation
C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub>	Homoserine		LA-CPFTFT spectrum
C <sub>4</sub> H <sub>10</sub> O <sub>4</sub>	Erythritol		LA-CPFT spectrum
C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	Glutamine		Angew.Chem.. 2019, 131,16148
C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	Arabinose		ms. in preparation
C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	Lixose		ms. in preparation
C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	Alanine-Glycine		LA-CPFT spectrum
C <sub>5</sub> H <sub>11</sub> NO	Norvaline		LA-CPFT spectrum
C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	Isovaline		ChemPhysChem 2020, 21,525
C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S	Methionine		ms. in preparation
C <sub>5</sub> H <sub>12</sub> O <sub>5</sub>	Arabitol		LA-CPFT spectrum
C <sub>5</sub> H <sub>12</sub> O <sub>5</sub>	Xylitol		ms. In preparation
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	Mannose		ms. in preparation
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	Allose		LA-CPFT spectrum
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	Manitol		LA-CPFT spectrum
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	Inositol		LA-CPFT spectrum
C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	Alanyl alanine		PCCP, 2020
C <sub>6</sub> H <sub>13</sub> N <sub>2</sub> O <sub>3</sub>	Cyclamic Acid		LA-CPFT spectrum
C <sub>7</sub> H <sub>12</sub> NSO <sub>3</sub>	Prolylglycine		LA-CPFT spectrum
C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	Mandelic acid		LA-CPFT spectrum
C <sub>8</sub> H <sub>8</sub> O <sub>4</sub>	Dopac		LA-CPFT spectrum

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>8</sub> H <sub>9</sub> NO <sub>3</sub>	Pyridoxal (Vit. B6)		ms. In preparation
C <sub>8</sub> H <sub>11</sub> NO <sub>3</sub>	Pyridoxine (Vit. B6)		ms. In preparation
C <sub>8</sub> H <sub>11</sub> NO <sub>3</sub>	Noradrenaline		ms. In preparation
C <sub>8</sub> H <sub>15</sub> NO <sub>6</sub>	N-Acetyl Glucosamine		LA-MB-FTMW spectrum
C <sub>9</sub> H <sub>11</sub> NO <sub>4</sub>	Dopa		LA-MB-FTMW spectrum
C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	Dulcine		ms. In preparation
C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>	Deoxyuridine		ms. In preparation
C <sub>9</sub> H <sub>13</sub> NO <sub>3</sub>	Adrenaline		ms. In preparation
C <sub>9</sub> H <sub>15</sub> NO	Pellirartine		LA-CPFT spectrum
C <sub>12</sub> H <sub>16</sub> N <sub>2</sub>	N,N-Dimethyltryptamine		ms. In preparation
C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	Sucrose		LA-CPFT spectrum
C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	Lactose		LA-CPFT spectrum
C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>	Testosterone		ms. In preparation

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In collaboration with:

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH <sub>5</sub> FO	Methylfluoride-H <sub>2</sub> O	Sharon Priya Gnanasekar Manuel Goubet, Robert Georges	Assigned transitions for hydrogen bond structure. Carbon bonded structure?
CH <sub>3</sub> 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?
C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub>	Acetonitrile-CO <sub>2</sub>	Sharon Priya Gnanasekar	Two structures, T-shaped and Stacked have been assigned For several isotopomers. Manuscript in preparation .
H <sub>4</sub> ArO <sub>2</sub>	Ar-(H <sub>2</sub> O) <sub>2</sub>	Arijit Das	A1 and B1 states of the trimer assigned and fitted. Earlier paper published in 2002 had assigned these states for Ar-(D <sub>2</sub> O) <sub>2</sub>
C <sub>3</sub> H <sub>5</sub> O <sub>2</sub>	propargyl alcohol-H <sub>2</sub> O	Sharon Priya Gnanasekar	Spectrum assigned for Several isotopomers. Manuscript in preparation

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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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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	Glutaronitrile	C. Cabezas, C. Bermúdez and J. Cernicharo	Accepted: A&A
C <sub>3</sub> H <sub>8</sub> S	Ethyl mehtyl sulfide (EMS)	C. Cabezas, C. Bermúdez and J. Cernicharo	Manuscript in Prep.
C <sub>3</sub> H <sub>6</sub> NO	N-ethylformamide	C. Bermúdez, C. Cabezas and J. Cernicharo	Manuscript in Prep.
C <sub>4</sub> H <sub>2</sub> N <sub>2</sub>	Maleonitrile	C. Bermúdez, C. Cabezas and J. Cernicharo	Assignment of ground state and vibrational excited states completed
CH <sub>4</sub> N <sub>2</sub>	Formamidine	C. Cabezas, C. Bermúdez and J. Cernicharo	Experiments in progress
C <sub>2</sub> H <sub>2</sub> O <sub>3</sub>	Formic anhydride	C. Bermúdez, C. Cabezas and J. Cernicharo	Experiments in progress

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

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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> , <b>123</b> (2019) 1091-1099.

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FORMULA	NAME OF COMPOUND	INVESTIGATORS	PRESENT STAGE OF PROGRESS
C <sub>3</sub> HN	cyanoacetylene	L. Bizzocchi, M. Melosso <sup>1</sup> , F. Tamassia <sup>2</sup> , O. Pirali <sup>3</sup> , M.A.-Martin Drumel <sup>3</sup> H.S.P. Müller <sup>4</sup> , et al.	Higher excited states IR/submm-wave ongoing
C <sub>3</sub> DN	<i>d</i> -cyanoacetylene	L. Bizzocchi, M. Melosso <sup>1</sup> , L. Dore <sup>1</sup> F. Tamassia <sup>2</sup> , A. Pietropolli- Charmet <sup>5</sup> , et al.	IR/submm-wave manuscript submitted to <i>JQSRT</i>
CD <sub>2</sub> S	thioformaldehyde- <i>d</i> <sub>2</sub>	V. Lattanzi et al.	mm-wave and submm-wave measurements completed
CHS <sub>2</sub> <sup>+</sup>	protonated carbon disulfide	V. Lattanzi, M.E. Palumbo <sup>7</sup> , M. McCarthy <sup>6</sup> , et al.	measurements ongoing
C <sub>2</sub> H <sub>4</sub> N <sub>2</sub>	<i>N</i> -cyano-methylamine	D. Prudenzano, J.-C. Guillemin <sup>8</sup> , M. Carvajal-Zaera <sup>9</sup> , et al.	measurements ongoing
CHN	Hydrogen isocyanide	L. Bizzocchi, S. Bailleux <sup>11</sup> , et al.	THz measurements ongoing
C <sup>15</sup> N	cyanogen radical	L. Bizzocchi, M. Melosso <sup>1</sup> , et al.	Measurements ongoing
CN <sup>+</sup>	cyanogen cation	V. Lattanzi, M. McCarthy <sup>6</sup> , et al.	Measurements ongoing
DHN	amidogen	L. Bizzocchi, M. Melosso <sup>1</sup> , L. Dore <sup>1</sup> , O. Pirali <sup>3</sup> , M.A.-Martin Drumel <sup>3</sup> , et al.	<i>ApJS.</i> , <b>247</b> , 59 (2020)
DH <sup>15</sup> N	<sup>15</sup> N-amidogen	L. Bizzocchi, M. Melosso <sup>1</sup> , L. Dore <sup>1</sup> , O. Pirali <sup>3</sup> , M.A.-Martin Drumel <sup>3</sup> , et al.	Measurements ongoing
C <sub>3</sub> H <sub>3</sub> N	Propargyl-imine	L. Bizzocchi, A. Pietropolli- Charmet <sup>5</sup> , J.-C. Guillemin <sup>8</sup> et al.	Manuscript submitted to <i>A&amp;A</i>

FORMULA	NAME OF COMPOUND	INVESTIGATORS	PRESENT STAGE OF PROGRESS
C <sub>2</sub> H <sub>4</sub> N	Allyl-imine	L. Bizzocchi, A. Pietropolli-Charmet <sup>5</sup> , et al.	E,Z isomers measurements completed
CH <sup>18</sup> O <sup>+</sup> , CH <sup>17</sup> O <sup>+</sup>	<sup>17,18</sup> O-carbonylium	L. Bizzocchi, et al.	THz measurements completed manuscript in preparation
ArH <sup>+</sup>	Argonium	L. Bizzocchi, M. Melosso <sup>1</sup> , et al.	Ar broadening THz measurements completed
C <sub>4</sub> H <sub>5</sub> N	Cyclopropyl cyanide	L. Bizzocchi, M. Melosso <sup>1</sup> , A. Pietropolli-Charmet <sup>5</sup> , et al.	FIR spectrum analysis ongoing
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	2-cyano-azyridine	L. Bizzocchi, J.-C. Guillemin <sup>8</sup> et al.	Measurements ongoing
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	Imidazole	B.M. Giuliano, L. Bizzocchi, A. Steber <sup>10</sup> , M. Schnell <sup>10</sup> , et al.	<i>A&amp;A</i> <b>628</b> , A59 (2019)

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
CH <sub>3</sub> I	Iodomethane	E. J. Juarez-Perez, <sup>1</sup> L. K. Ono, <sup>1</sup> I. Uriarte, E. J. Cocinero Y. Qi <sup>1</sup>	<i>ACS Appl. Mater. Interfaces</i> , <b>11</b> , 12586 (2019) <a href="https://doi.org/10.1021/acsami.9b02374">https://doi.org/10.1021/acsami.9b02374</a>
CH <sub>3</sub> NH <sub>2</sub>	Methylamine	E. J. Juarez-Perez, <sup>1</sup> L. K. Ono, <sup>1</sup> I. Uriarte, E. J. Cocinero Y. Qi <sup>1</sup>	<i>ACS Appl. Mater. Interfaces</i> , <b>11</b> , 12586 (2019) <a href="https://doi.org/10.1021/acsami.9b02374">https://doi.org/10.1021/acsami.9b02374</a>
CH <sub>9</sub> ClF <sub>3</sub> NO [CClF <sub>3</sub> ···N(CH <sub>3</sub> ) <sub>3</sub> ]	trifluorochloromethane···trimethylammonia	Caminati's group <sup>2</sup> Cocinero's group	Analysis in progress.
C <sub>2</sub> Cl <sub>4</sub> F <sub>2</sub> [CCl <sub>2</sub> FCCL <sub>2</sub> F]	CFC 112a	Cocinero's group Kisiel's group <sup>3</sup>	1 conformer assigned.
C <sub>2</sub> H <sub>6</sub> F <sub>2</sub> O <sub>2</sub>	(Difluoromethane)···(Water) <sub>2</sub>	C. Calabrese, W. Li, <sup>2</sup> G. Prampolini, <sup>4</sup> L. Evangelisti, <sup>2</sup> I. Uriarte, I. Cacelli, <sup>4</sup> S. Melandri, <sup>2</sup> E. J. Cocinero	<i>Angew. Chem. Int. Ed.</i> , <b>131</b> , 8525-8530 (2019) <a href="https://doi.org/10.1002/ange.201902753">https://doi.org/10.1002/ange.201902753</a> 'Paper of the month' by SBE
C <sub>2</sub> H <sub>6</sub> F <sub>2</sub> O <sub>3</sub>	(Difluoromethane)···(Water) <sub>3</sub>	C. Calabrese, W. Li, <sup>2</sup> G. Prampolini, <sup>4</sup> L. Evangelisti, <sup>2</sup> I. Uriarte, I. Cacelli, <sup>4</sup> S. Melandri, <sup>2</sup> E. J. Cocinero	<i>Angew. Chem. Int. Ed.</i> , <b>131</b> , 8525-8530 (2019) <a href="https://doi.org/10.1002/ange.201902753">https://doi.org/10.1002/ange.201902753</a> 'Paper of the month' by SBE
C <sub>4</sub> H <sub>6</sub> F <sub>4</sub> O	(Difluoromethane) <sub>2</sub> ···(Water)	C. Calabrese, W. Li, <sup>2</sup> G. Prampolini, <sup>4</sup> L. Evangelisti, <sup>2</sup> I. Uriarte, I. Cacelli, <sup>4</sup> S. Melandri, <sup>2</sup> E. J. Cocinero	<i>Angew. Chem. Int. Ed.</i> , <b>131</b> , 8525-8530 (2019) <a href="https://doi.org/10.1002/ange.201902753">https://doi.org/10.1002/ange.201902753</a> 'Paper of the month' by SBE



C <sub>4</sub> H <sub>8</sub> F <sub>4</sub> O <sub>2</sub>	(Difluoromethane) <sub>2</sub> ⋯(Water) <sub>2</sub>	C. Calabrese, W. Li, <sup>2</sup> G. Prampolini, <sup>4</sup> L. Evangelisti, <sup>2</sup> I. Uriarte, I. Cacelli, <sup>4</sup> S. Melandri, <sup>2</sup> E. J. Cocinero	<b>Angew. Chem. Int. Ed.</b> , <u>131</u> , 8525-8530 (2019) <a href="https://doi.org/10.1002/ange.201902753">https://doi.org/10.1002/ange.201902753</a> 'Paper of the month' by SBE
C <sub>10</sub> H <sub>10</sub> F <sub>10</sub>	(Difluoromethane) <sub>5</sub>	Cocinero's group Melandri's group <sup>2</sup> Pate's group <sup>5</sup>	1 complex assigned. <i>Manuscript in preparation.</i>
C <sub>12</sub> H <sub>12</sub> F <sub>12</sub>	(Difluoromethane) <sub>6</sub>	Cocinero's group Melandri's group <sup>2</sup> Pate's group <sup>5</sup>	2 complexes assigned. <i>Manuscript in preparation.</i>
C <sub>14</sub> H <sub>14</sub> F <sub>14</sub>	(Difluoromethane) <sub>7</sub>	Cocinero's group Melandri's group <sup>2</sup> Pate's group <sup>5</sup>	1 complex assigned. <i>Manuscript in preparation.</i>
C <sub>2</sub> H <sub>6</sub> OS	Dimethyl sulfoxide (DMSO)	Cocinero's group	Analysis in progress.
C <sub>2</sub> H <sub>8</sub> O <sub>2</sub> S	Dimethyl sulfoxide (DMSO)⋯(Water)	Cocinero's group	Analysis in progress.
C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>2</sub> O [CHCl <sub>2</sub> CF <sub>2</sub> OCH <sub>3</sub> ]	Methoxyflurane	Lesarri's group <sup>6</sup> Cocinero's group Grabow's group <sup>7</sup>	Analysis in progress.
C <sub>4</sub> H <sub>8</sub> O <sub>4</sub>	Erythrose	Cocinero's group	1 conformer + <sup>13</sup> C assigned. <i>Manuscript in preparation.</i>
C <sub>6</sub> H <sub>5</sub> ClF <sub>3</sub> N	Pyridine⋯chlorotrifluoromethane	Gou's group <sup>8</sup> Caminati's group <sup>2</sup> Cocinero's group	<i>Manuscript Submitted</i>
C <sub>9</sub> H <sub>15</sub> NO	Pyridine⋯ <i>tert</i> -butyl alcohol	L. Spada, <sup>2</sup> I. Uriarte, W. Li, <sup>2</sup> L. Evangelisti, <sup>2</sup> E. J. Cocinero W. Caminati <sup>2</sup>	<b>Phys. Chem. Chem. Phys.</b> , <u>21</u> , 3545-3549 (2019) <a href="https://doi.org/10.1039/C8CP04462G">https://doi.org/10.1039/C8CP04462G</a>
C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	Lyxose	C. Calabrese, P. Écija, I. Compañón, M. Vallejo-López, Á. Cimas, M. Parra, F. J. Basterretxea, J. I. Santos, J. Jiménez-Barbero, A. Lesarri, F. Corzana <sup>9</sup> E. J. Cocinero	<b>J. Phys. Chem. Lett.</b> , <u>10</u> , 3339-3345 (2019) <a href="https://doi.org/10.1021/acs.jpcllett.9b00978">https://doi.org/10.1021/acs.jpcllett.9b00978</a>
C <sub>10</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>	(Prolinol) <sub>2</sub>	Cocinero's group Sanz's group <sup>10</sup>	Homodimer RR/SS assigned.
C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>	Glucoronolactone	Cocinero's group	2 conformers.
C <sub>6</sub> H <sub>10</sub> O <sub>7</sub>	Glucuronic acid	Cocinero's group	2 conformers. <i>Manuscript in preparation.</i>
C <sub>6</sub> H <sub>10</sub> O <sub>7</sub>	Galacturonic acid	Cocinero's group	1 conformer. <i>Manuscript in preparation.</i>
C <sub>6</sub> H <sub>12</sub> O	Oxacycloheptene	Lesarri's group <sup>6</sup> Grabow's group <sup>7</sup> Cocinero's group	Analysis in progress.
C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	Fucose	Cocinero's group	1 conformer – <sup>13</sup> Cs assigned.
C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	Rhamnose	Cocinero's group	1 conformer assigned.

$C_6H_{12}O_4$ [CH <sub>2</sub> (OH)CH <sub>2</sub> (CHOH) <sub>2</sub> COCH <sub>3</sub> ]	Methyl- $\alpha$ -2-deoxyribofuranoside	C. Calabrese, I. Uriarte, A. Insausti, M. Vallejo-López, F. J. Basterretxea, S. A. Cochrane, B. G. Davis, <sup>11</sup> F. Corzana, <sup>9</sup> E. J. Cocinero	<b>ACS Cent. Sci.</b> <u>6</u> , 293-303, (2020) <a href="https://doi.org/10.1021/acscentsci.9b01277">https://doi.org/10.1021/acscentsci.9b01277</a> Journal cover 'Paper of the month' by SBE
$C_6H_{12}O_4$ [CH <sub>2</sub> (OH)CH <sub>2</sub> (CHOH) <sub>2</sub> COCH <sub>3</sub> ]	Methyl- $\beta$ -2-deoxyribofuranoside	C. Calabrese, I. Uriarte, A. Insausti, M. Vallejo-López, F. J. Basterretxea, S. A. Cochrane, B. G. Davis, <sup>11</sup> F. Corzana, <sup>9</sup> E. J. Cocinero	<b>ACS Cent. Sci.</b> <u>6</u> , 293-303, (2020) <a href="https://doi.org/10.1021/acscentsci.9b01277">https://doi.org/10.1021/acscentsci.9b01277</a> Journal cover 'Paper of the month' by SBE
$C_6H_{12}O_4$ [CH <sub>2</sub> (OH)CH <sub>2</sub> (CHOH) <sub>2</sub> COCH <sub>3</sub> ]	Methyl- $\alpha$ -2-deoxyribofuranoside	C. Calabrese, I. Uriarte, A. Insausti, M. Vallejo-López, F. J. Basterretxea, S. A. Cochrane, B. G. Davis, <sup>11</sup> F. Corzana, <sup>9</sup> E. J. Cocinero	<b>ACS Cent. Sci.</b> <u>6</u> , 293-303, (2020) <a href="https://doi.org/10.1021/acscentsci.9b01277">https://doi.org/10.1021/acscentsci.9b01277</a> Journal cover 'Paper of the month' by SBE
$C_6H_{12}O_4$ [CH <sub>2</sub> (OH)CH <sub>2</sub> (CHOH) <sub>2</sub> COCH <sub>3</sub> ]	Methyl- $\beta$ -2-deoxyribofuranoside	C. Calabrese, I. Uriarte, A. Insausti, M. Vallejo-López, F. J. Basterretxea, S. A. Cochrane, B. G. Davis, <sup>11</sup> F. Corzana, <sup>9</sup> E. J. Cocinero	<b>ACS Cent. Sci.</b> <u>6</u> , 293-303, (2020) <a href="https://doi.org/10.1021/acscentsci.9b01277">https://doi.org/10.1021/acscentsci.9b01277</a> Journal cover 'Paper of the month' by SBE
$C_6H_{11}FO_5$	2-fluoro-2-deoxy-glucose	Cocinero's group	2 conformers assigned. <i>Manuscript in preparation.</i>
$C_6H_{11}FO_5$	2-fluoro-2-deoxy-mannose	Cocinero's group	2 conformers assigned. <i>Manuscript in preparation.</i>
$C_6H_{11}FO_5$	2-fluoro-2-deoxy-galactose	Cocinero's group	1 conformer assigned. <i>Manuscript in preparation.</i>
$C_6H_{12}O_5$	2-deoxyglucose	Cocinero's group	3 conformers assigned <i>Manuscript in preparation.</i>
$C_6H_{12}O_5$	2-deoxygalactose	Cocinero's group	2 conformers – 13Cs assigned <i>Manuscript in preparation.</i>
$C_7H_6N_2$	Indazole	I. Uriarte, F. Reviriego, C. Calabrese, J. Elguero, <sup>12</sup> Z. Kisiel, <sup>3</sup> I. Alkorta, <sup>12</sup> E. J. Cocinero	<b>Chem. Eur. J.</b> <u>25</u> , 10172-10178, (2019). <a href="https://doi.org/10.1002/chem.201901666">https://doi.org/10.1002/chem.201901666</a>
$C_7H_{17}NO_5$	N-Methyl-glucamine	Cocinero's group	1 conformed assigned
$C_8H_8O_2$	Methyl benzoate	Cocinero's group	1 conformer -13Cs -18Os assigned
$C_8H_{10}O_3$	Methyl benzoate···water	Cocinero's group	2 conformer -13Cs - assigned
$C_8H_{12}O_4$	Methyl benzoate···(water) <sub>2</sub>	Cocinero's group	2 conformers assigned
$C_8H_{14}O_5$	Methyl benzoate···(water) <sub>3</sub>	Cocinero's group	2 conformers assigned
$C_8H_{16}O_6$	Methyl benzoate···(water) <sub>4</sub>	Cocinero's group	2 conformers assigned
$C_{16}H_{16}O_4$	(Methyl benzoate) <sub>2</sub>	Cocinero's group	1 complex assigned

C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> [C <sub>6</sub> H <sub>5</sub> CHCHCOOCH <sub>3</sub> ]	Methyl cinnamate	Cocinero's group Lesarri's group <sup>6</sup>	2 conformers assigned
C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	Dimethyl phthalate	Cocinero's group	1 conformer - <sup>13</sup> Cs assigned
C <sub>10</sub> H <sub>12</sub> O <sub>3</sub> [HOCH <sub>2</sub> CH(OCH <sub>3</sub> )CHCH <sub>2</sub> OH]	Coniferyl alcohol	Cocinero's group Lesarri's group <sup>6</sup>	Analysis in progress.
C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub> [NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> COO(CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub> ]	Butamben	A. Insausti, C. Calabrese, M. Parra, I. Usabiaga, M. Vallejo-López P. Écija, F. J. Basterretxea, J.-U. Grabow, <sup>7</sup> A. Lesarri, <sup>6</sup> W. Caminati, <sup>2</sup> E. J. Cocinero	<b>Chem. Comm.</b> Accepted manuscript, (2020). <a href="https://doi.org/10.1039/DOCC00760A">https://doi.org/10.1039/DOCC00760A</a>
C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub> [NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> COOCH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]	Isobutamben	A. Insausti, C. Calabrese, M. Parra, I. Usabiaga, M. Vallejo-López P. Écija, F. J. Basterretxea, J.-U. Grabow, <sup>7</sup> A. Lesarri, <sup>6</sup> W. Caminati, <sup>2</sup> E. J. Cocinero	<b>Chem. Comm.</b> Accepted manuscript, (2020). <a href="https://doi.org/10.1039/DOCC00760A">https://doi.org/10.1039/DOCC00760A</a>
C <sub>12</sub> H <sub>22</sub> O <sub>2</sub>	Oxacyclotridecan-2-one	Cocinero's group	22 conformers - <sup>13</sup> Cs assigned
C <sub>15</sub> H <sub>12</sub> O <sub>2</sub> [C <sub>6</sub> H <sub>5</sub> COCH <sub>2</sub> COC <sub>6</sub> H <sub>5</sub> ]	Dibenzoylmethane	Cocinero's group Caminati's group <sup>2</sup>	1 conformer assigned
C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>	16-Hexadecanolide	Cocinero's group	1 conformer assigned

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
O <sub>3</sub> U	Uranium (VI) oxide	B. E. Long <sup>†</sup>	Spectrum observed.
O <sub>2</sub> Th	Thorium (IV) oxide	B. E. Long <sup>†</sup>	Spectrum observed.
C <sub>4</sub> H <sub>9</sub> F	2H-Nonafluorobutane		Parent and minor isotopologues observed and assigned
C <sub>5</sub> Cl <sub>2</sub> F <sub>6</sub>	1,2-dichlorohexafluorocyclopentene-1		Spectrum assigned
C <sub>6</sub> Cl <sub>2</sub> F <sub>8</sub>	1,2-dichlorooctafluorocyclohexene-1		Spectrum assigned
C <sub>3</sub> F <sub>5</sub> ClO	Chloropentafluoroacetone	W. C. Bailey <sup>Δ</sup>	Manuscript in preparation
C <sub>3</sub> F <sub>4</sub> Cl <sub>2</sub> O	1,3-Dichlorotetrafluoroacetone		Manuscript in preparation
C <sub>3</sub> H <sub>2</sub> F <sub>3</sub> ClO	1,1,1-Trifluoro-3-chloroacetone		Manuscript in preparation
C <sub>3</sub> H <sub>4</sub> F <sub>2</sub> O	1,1-Difluoroacetone	P. Groner <sup>‡</sup> L. Margulès, R. Motiyenko <sup>§</sup>	CP-FTMW Spectrum Assigned mmW spectrum recorded.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>3</sub> H <sub>5</sub> ClO	Chloroacetone	B. E. Long <sup>†</sup>	Spectrum assigned
C <sub>3</sub> F <sub>5</sub> N	Perfluoropropionitrile	B. E. long <sup>†</sup>	Spectrum Assigned
BaS	Barium Monosulfide	G. S. Grubbs II <sup>•</sup>	Hyperfine structure, J = 1 - 0, 2 - 1 in high vibrational states.
C <sub>3</sub> F <sub>6</sub> NH	Hexafluoroacetone imine	G. S. Grubbs II <sup>•</sup> , D. Obenchain <sup>††</sup> , D. Frohman, S. E. Novick <sup>†</sup> , W. C. Pringle <sup>†</sup>	Spectrum assigned
C <sub>4</sub> F <sub>9</sub> I	Perfluoroiodobutane	G. S. Grubbs II <sup>•</sup> , R. Bohn <sup>♦</sup>	Manuscript in preparation
C <sub>4</sub> H <sub>6</sub> F <sub>3</sub> I	3-Iodo-1,1,1-trifluorobutane	W. C. Bailey <sup>Δ</sup>	CP-FTMW spectrum assigned
C <sub>3</sub> HF <sub>7</sub> O	1,2,2,2-Tetrafluoroethyl trifluoromethyl ether	A. Turk	Spectrum assigned
C <sub>5</sub> H <sub>3</sub> F <sub>7</sub> O <sub>2</sub>	2,2,3,3-Tetrafluoropropyl trifluoroacetate		Spectrum assigned
C <sub>4</sub> H <sub>7</sub> ClF <sub>2</sub> O	1-chloro-1,1-difluoro-2-methyl-2-propanol		Spectrum assigned
C <sub>3</sub> H <sub>4</sub> F <sub>3</sub> I	1,1,1-trifluoro-3-iodopropane	W. C. Bailey <sup>Δ</sup>	Manuscript in preparation
C <sub>3</sub> H <sub>2</sub> F <sub>5</sub> I	1,1,1,2,2-pentafluoro-3-iodopropane	W. C. Bailey <sup>Δ</sup>	Manuscript in preparation
C <sub>10</sub> F <sub>19</sub> N	Perfluorodecanonitrile	A. J. Minei <sup>□</sup>	Spectrum observed
C <sub>3</sub> H <sub>6</sub> F <sub>3</sub> N	1,1,1-Trifluoro-3-azapent-3-ene	C. T. Dewberry <sup>*</sup>	Spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>5</sub> H <sub>11</sub> F	1-Fluoropentane	D. Obenchain <sup>⊥+</sup>	Spectrum Assigned
C <sub>6</sub> H <sub>13</sub> F	1-Fluorohexane	D. Obenchain <sup>⊥+</sup>	Spectrum Assigned
C <sub>7</sub> H <sub>15</sub> F	1-Fluoroheptane	D. Obenchain <sup>⊥+</sup>	Spectrum Assigned
C <sub>8</sub> H <sub>17</sub> F	1-Fluorooctane	D. Obenchain <sup>⊥+</sup> , W. Orellana <sup>⊥</sup>	Spectrum Assigned
C <sub>5</sub> H <sub>12</sub> S	Butyl methyl thioether	J. Ogulnick, T. Holmes	Spectrum Assigned
C <sub>6</sub> H <sub>14</sub> S	Pentyl methyl thioether	J. Ogulnick, T. Holmes	Spectrum Assigned

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Formula	Name of Compound	Name of Investigator(s)	Present Stage of Progress
CCl <sub>2</sub> O (COCl <sub>2</sub> )	Carbonyl chloride (phosgene)	Drouin <sup>1</sup>	Millimeter wave spectra analyzed, spectra for mixed isotopomer
CDH <sub>3</sub> O (CH <sub>2</sub> DOH)	Deuterated Methanol	Pearson <sup>1</sup> , Yu <sup>1</sup> , & Drouin <sup>1</sup>	Ext. J,K analysis in progress
CHN (HCN)	Hydrogen cyanide	Pearson <sup>1</sup> , Yu <sup>1</sup> , & Cernicharo <sup>2</sup>	Vib. Excited rotational data recorded, analyzed
CH <sub>3</sub> NO <sub>3</sub>	Methyl nitrate	Drouin <sup>1</sup> , & Zhang <sup>1</sup>	Submm data acquired, assigned
C <sub>3</sub> H <sub>9</sub> NO	Alaninol	Crawford <sup>1,3</sup> & Yu <sup>1</sup>	75-110 GHz mm data recorded
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	Glycidol	Liu <sup>1,4</sup> & Yu <sup>1</sup>	75-110 GHz mm data recorded
CH <sub>4</sub>	Methane	Drouin <sup>1</sup>	2.5-2.7 THz spectra for <sup>12</sup> C, <sup>13</sup> C
C <sub>5</sub> H <sub>8</sub>	Isoprene	Drouin <sup>1</sup> , Kisiel <sup>5</sup> , Porterfield <sup>6</sup> , & Martin <sup>7</sup>	100-300 GHz spectra collected, analysis in progress
ClH (HCl)	Hydrogen Chloride	Gupta <sup>1,8</sup> , Drouin <sup>1</sup> , & Pearson <sup>1</sup>	THz spectra to v=8
ClO	Chlorine Monoxide	Cohen <sup>1</sup> , Drouin <sup>1</sup> , & Duffy <sup>9</sup>	Rotational data to v=8, analysis complete
CH <sub>2</sub> <sup>+</sup> (H <sub>2</sub> Cl <sup>+</sup> )	Chloronium	Gupta <sup>1,8</sup> , Drouin <sup>1</sup> , & Pearson <sup>1</sup>	THz spectra recorded
CO <sub>2</sub>	Carbon Dioxide ( <sup>18</sup> OCO)	Drouin <sup>1</sup> , & Elliot <sup>1,10</sup>	Isotopic measurements 0.5-0.6 THz
C <sub>2</sub> DH (HCCD)	Deuterated Acetylene	Yu <sup>1</sup> , Drouin <sup>1</sup> , & Walters <sup>11</sup>	THz spectra measured, assigned
C <sub>3</sub> H <sub>5</sub> N (CH <sub>3</sub> CH <sub>2</sub> CN)	Propionitrile (ethyl cyanide)	Pearson <sup>1</sup> , Daly <sup>1,12</sup> , Alonzo <sup>13</sup> , & Yu <sup>1</sup>	Excited vibrational analyses in progress
H <sup>15</sup> NO <sub>2</sub>	Nitrous Acid	Drouin <sup>1</sup> & Miller <sup>1</sup>	Submillimeter spectra recorded, assigned
HO <sub>2</sub>	Hydroperoxyl radical	Drouin <sup>1</sup>	N <sub>2</sub> and O <sub>2</sub> temperature dependent pressure broadening
H <sub>2</sub> O	Water ( <sup>17</sup> O & <sup>18</sup> O)	Yu <sup>1</sup> , Drouin <sup>1</sup> , Pearson <sup>1</sup> , & Walters <sup>11</sup>	Measurements through 2.6 THz for <sup>18</sup> O and 2.7THz for <sup>17</sup> O
H <sub>2</sub> N	Amidogen	Müller <sup>14</sup> & Drouin <sup>1</sup>	Gs analysis complete, excited vibrational state analysis in progress

Formula	Name of Compound	Name of Investigator(s)	Present Stage of Progress
O <sub>2</sub>	Molecular oxygen	Vogt <sup>15</sup> , Kerber <sup>16</sup> , Mehner <sup>15</sup> , Yu <sup>1</sup> , Pfrommer <sup>16</sup> , Curto <sup>15</sup> , et al.	Rotational Raman line frequencies calculated and provided in Supp. material, Phys. Rev. Lett. <b>123</b> (2019), 061101
O <sub>2</sub> S (SO <sub>2</sub> )	Sulfur Dioxide	Drouin <sup>1</sup>	Temperature dependent air pressure broadening

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
H <sub>4</sub> O <sub>2</sub> (H <sub>2</sub> O-H <sub>2</sub> O)	water dimer	W. Caminati et al.	High J, high K transitions observed
CClF <sub>3</sub> Kr (CCl <sub>3</sub> -Kr)	chlorotrifluoromethane krypton	L. Evangelisti	Asymmetric top spectrum
CH <sub>2</sub> CIFNe (CH <sub>2</sub> CIF-Ne)	chlorofluoromethane neon	P. Ottaviani et al. ISMN	Spectrum observed, dynamics
CH <sub>2</sub> F <sub>2</sub> Ne (CH <sub>2</sub> F <sub>2</sub> -Ne)	difluoromethane neon	S. Melandri et al.	Spectrum assigned, dynamics
CH <sub>3</sub> F <sub>4</sub> N (CF <sub>4</sub> -NH <sub>3</sub> )	tetrafluoromethane ammonia	L. Evangelisti et al.	Symmetric top, tunneling
CH <sub>4</sub> F <sub>3</sub> N (CHF <sub>3</sub> -H <sub>3</sub> N)	trifluoromethane ammonia	B.M. Giuliano et al.	mmw measurements
CH <sub>6</sub> O <sub>2</sub> (CH <sub>3</sub> OH-H <sub>2</sub> O)	methanol water	S. Melandri et al.	High J, high K transitions observed
C <sub>2</sub> F <sub>4</sub> O (CF <sub>4</sub> -CO)	tetrafluoromethane carbon monoxide	L. Evangelisti et al.	Spectrum assigned, symmetric top
C <sub>2</sub> F <sub>3</sub> KrN (C <sub>2</sub> F <sub>3</sub> N-Kr)	trifluoroacetonitrile krypton	L. Evangelisti et al.	Symmetric top
C <sub>2</sub> H <sub>2</sub> F <sub>4</sub> O (C <sub>2</sub> F <sub>4</sub> -H <sub>2</sub> O)	tetrafluoroethene water	Q. Gou et al. CQU	Spectrum recorded
C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> Cl <sub>2</sub> (CH <sub>3</sub> Cl-CF <sub>3</sub> Cl)	chloromethane chlorotrifluoromethane	W. Li et al.	Spectrum assigned
C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O (CHF <sub>3</sub> -CH <sub>2</sub> O)	trifluoromethane formaldehyde	Q. Gou et al. UVA, UPV, CQU	1 conformer, 4 states
C <sub>2</sub> H <sub>4</sub> NeO (C <sub>2</sub> H <sub>4</sub> 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
$C_3H_6O_3$ ( $C_3H_4O_2-H_2O$ )	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
$C_3H_7NO_2$ ( $C_3H_5NO - H_2O$ )	Acrylamide - water	A. Maris et al. - UVA	Spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub> (C <sub>3</sub> H <sub>5</sub> NO <sub>2</sub> -H <sub>2</sub> O)	1,3-oxazolidin-2-one Water	A. Maris et al.	Spectrum assigned, tunnelling
C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O	N,N'-dimethylurea	A. Maris et al.	Spectrum recorded
C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> (C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O-H <sub>2</sub> O)	Ethyleneurea Water	A. Maris et al.	Spectrum assigned
C <sub>4</sub> H <sub>4</sub> O <sub>4</sub> (C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> -CO <sub>2</sub> )	acrylic acid carbon dioxide	A. Maris	2 conformers assigned
C <sub>4</sub> H <sub>4</sub> F <sub>4</sub> O <sub>4</sub>	<i>alpha, alpha</i> -difluoroacetic acid dimer	Q. Gou et al. CQU	4 states, proton tunneling
C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> (C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> -CH <sub>2</sub> O <sub>2</sub> )	<i>beta</i> -propiolactone formic acid	L. Evangelisti et al. UVA	Spectrum assigned
C <sub>4</sub> H <sub>6</sub> F <sub>4</sub> O (C <sub>2</sub> H <sub>6</sub> O-C <sub>2</sub> F <sub>4</sub> )	dimethylether tetrafluoroethene	L. Evangelisti et al.	Spectrum recorded
C <sub>4</sub> H <sub>7</sub> NO	2-pyrrolidinone	A. Maris et al.	Spectrum assigned, ND species
C <sub>4</sub> H <sub>7</sub> NO	metacrylamide	A. Maris et al.	Spectrum assigned, MS in prep.
C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub>	3-methyl-1,3-oxazolidin-2- one	A. Maris et al.	Spectrum assigned, tunnelling, V <sub>3</sub>
C <sub>4</sub> H <sub>8</sub> O	1-methylcyclopropanol	W. Li et al.	Spectrum assigned, tunneling
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	isopropylformate	L. Spada et al. ISMN	Spectrum assigned
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	Acroleine - methanol	D. Lv et al.	Spectrum assigned
C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> (C <sub>4</sub> H <sub>7</sub> NO-H <sub>2</sub> O)	2-pyrrolidinone Water	A. Maris et al.	Spectrum assigned, ND species
C <sub>4</sub> H <sub>12</sub> O <sub>4</sub> (C <sub>6</sub> H <sub>18</sub> O <sub>6</sub> )	Ethylene glycol dimer (and trimer)	Usabiaga et al. UVA	Spectrum assigned
C <sub>4</sub> D <sub>8</sub> O	tetrahydrofuran- <i>d</i> <sub>8</sub>	A. Maris et al. UVA, RM	Pseudorotation splittings
C <sub>4</sub> H <sub>9</sub> ClF <sub>3</sub> N (CClF <sub>3</sub> -C <sub>3</sub> H <sub>9</sub> N)	chlorotrifluoromethane trimethylamine	L. Evangelisti et al. UPV	Halogen bond
C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> (C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ) <sub>2</sub>	Nitroethane dimer	W. Li et al.	Spectrum recorded
C <sub>4</sub> H <sub>10</sub> O <sub>3</sub>	trimethoxymethane	G. Feng et al. LISA	3 conformers assigned
C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>	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 <sub>5</sub> H <sub>3</sub> F <sub>4</sub> NO (C <sub>5</sub> HF <sub>4</sub> N-H <sub>2</sub> O)	2,3,4,6-trifluoropyridine Water	C. Calabrese et al.	Spectrum assigned, MS in prep.
C <sub>5</sub> H <sub>4</sub> F <sub>3</sub> NO (C <sub>5</sub> H <sub>2</sub> F <sub>3</sub> N-H <sub>2</sub> O)	2,4,6-trifluoropyridine Water	C. Calabrese et al.	Spectrum assigned, MS in prep.
C <sub>5</sub> H <sub>5</sub> F <sub>2</sub> NO (C <sub>5</sub> H <sub>3</sub> F <sub>2</sub> N-H <sub>2</sub> O)	3,5-difluoropyridine Water	C. Calabrese et al.	Spectrum assigned, MS in prep.
C <sub>5</sub> H <sub>5</sub> F <sub>2</sub> NO (C <sub>5</sub> H <sub>3</sub> F <sub>2</sub> N-H <sub>2</sub> O)	2,6-difluoropyridine Water	C. Calabrese et al.	Spectrum assigned, MS in prep.
C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	acetylacetone	W. Caminati et al. PCI, KU	Spectrum observed
C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	Acrolein - ethanol	D. Lv et al.	Spectrum assigned
C <sub>5</sub> H <sub>10</sub> O <sub>3</sub> (C <sub>4</sub> H <sub>8</sub> O-CH <sub>2</sub> O <sub>2</sub> ) (C <sub>4</sub> H <sub>8</sub> O-CHDO <sub>2</sub> )	1-methylcyclopropanol formic acid	W. Li et al.	Spectrum assigned
C <sub>5</sub> H <sub>12</sub> O	2-methyl-2-butanol	L. Spada et al. ISMN	5 conformers assigned
C <sub>5</sub> H <sub>12</sub> O <sub>3</sub> (CH <sub>2</sub> O <sub>2</sub> -C <sub>4</sub> H <sub>10</sub> O)	formic acid <i>tert</i> -butanol	L. Evangelisti et al.	Spectrum assigned, tunneling
C <sub>6</sub> F <sub>5</sub> NO (C <sub>5</sub> F <sub>5</sub> N-CO)	Pentafluoropyridine CO	S. Melandri et al.	Spectrum assigned
C <sub>6</sub> H <sub>3</sub> F <sub>2</sub> N (C <sub>5</sub> F <sub>5</sub> N-CFH <sub>3</sub> )	Pentafluoropyridine fluoromethane	S. Melandri et al.	Spectrum assigned
C <sub>6</sub> H <sub>3</sub> F <sub>6</sub> N (C <sub>6</sub> F <sub>6</sub> -NH <sub>3</sub> ) (C <sub>6</sub> F <sub>6</sub> - <sup>15</sup> NH <sub>3</sub> )	hexafluorobenzene ammonia	S. Melandri et al. ISMN	Spectrum assigned
C <sub>6</sub> H <sub>5</sub> ClF <sub>3</sub> N (C <sub>5</sub> H <sub>5</sub> N-CClF <sub>3</sub> )	pyridine chlorotrifluoromethane	Q. Gou et al. CQU	Halogen bond
C <sub>6</sub> H <sub>7</sub> NO <sub>2</sub> S	benzenesulfonamide	S. Melandri et al. KCL	Spectrum assigned, ND species
C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S	sulfanilamide	A. Vigorito et al. KCL	Spectrum assigned
C <sub>6</sub> H <sub>9</sub> NO (C <sub>5</sub> H <sub>5</sub> N-CH <sub>4</sub> O)	pyridine methanol	L. Evangelisti et al.	Spectrum assigned
C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> (C <sub>3</sub> H <sub>5</sub> N-C <sub>3</sub> H <sub>5</sub> N)	propargylamine dimer	L. Spada et al. UBO	Spectrum assigned
C <sub>6</sub> H <sub>10</sub> O	<i>Trans</i> -2-Hexen-1-al	L. Evangelisti et al. UVA	Spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>12</sub> F <sub>3</sub> N (C <sub>5</sub> H <sub>11</sub> N-CHF <sub>3</sub> )	<i>N</i> -methylpyrrolidine trifluoromethane	L. Evangelisti et al.	H-bond, internal rotation
C <sub>6</sub> H <sub>12</sub> O	<i>cyclo</i> -hexanol	W. Li et al. UVA	2 conformers assigned
C <sub>6</sub> H <sub>12</sub> O	<i>Cis</i> -3hexen-1-ol	L. Evangelisti et al. UVA	2 conformers assigned
C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	<i>trans</i> -1,2-cyclohexanediol	W. Caminati et al.	Spectrum assigned, OD species
C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> (C <sub>2</sub> H <sub>6</sub> O-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> )	ethanol 1,4-dioxane	L. Evangelisti et al.	1 conformer observed
C <sub>7</sub> F <sub>6</sub> O (C <sub>6</sub> F <sub>6</sub> -CO)	hexafluorobenzene carbon monoxide	S. Melandri et al. ISMN	Spectrum assigned
C <sub>7</sub> H <sub>6</sub> F <sub>2</sub> O	2,6-difluorobenzylalcohol	L. Evangelisti et al.	Spectrum assigned, tunnelling
C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> S	<i>p</i> -toluenesulfonamide	C. Calabrese et al. KCL	3 species assigned
C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> S	<i>o</i> -toluenesulfonamide	A. Vigorito et al. KCL	Spectrum assigned, V <sub>3</sub>
C <sub>7</sub> H <sub>11</sub> NO (C <sub>7</sub> H <sub>9</sub> N-H <sub>2</sub> O)	benzylamine water	S. Melandri et al.	1 conformer
C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	3,5-heptanedione	L. Evangelisti et al.	2 conformers
C <sub>7</sub> H <sub>14</sub> O <sub>3</sub> (C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> -H <sub>2</sub> O)	3,5-heptanedione Water	W. Li et al.	2 conformers
C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	<i>cyclo</i> -hexylformate	L. Evangelisti et al.	1 conformer
C <sub>8</sub> H <sub>8</sub> O	<i>p</i> -tolualdehyde	W. Caminati et al. PCI, LISA, NIST	V <sub>3</sub> & V <sub>6</sub>
C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	phenyl acetate	W. Caminati et al.	Spectrum assigned
C <sub>8</sub> H <sub>10</sub> FN	<i>p</i> -fluorophenylethylamine	S. Melandri et al.	2 conformers assigned
C <sub>8</sub> H <sub>16</sub> O	1-octen-3-ol	A. Maris et al.	2 conformers assigned
C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> (C <sub>4</sub> H <sub>9</sub> N-C <sub>4</sub> H <sub>9</sub> N)	pyrrolidine dimer	A. Maris et al. ISMN	Spectrum assigned
C <sub>9</sub> H <sub>9</sub> F <sub>6</sub> N (C <sub>6</sub> F <sub>6</sub> -N(CH <sub>3</sub> ) <sub>3</sub> )	Hexafluorobenzene Trimetilammina	W. Li et al.	Spectrum assigned
C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	eugenol	A. Maris et al.	Spectrum assigned
C <sub>13</sub> H <sub>13</sub> F <sub>6</sub> N (C <sub>6</sub> F <sub>6</sub> -C <sub>7</sub> H <sub>13</sub> 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, Zufikon (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)
UBO	Department of Chemistry, University of Bologna (I)

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>5</sub> H <sub>11</sub> NO (HCONHC(CH <sub>3</sub> ) <sub>3</sub> )	N-tert-Butylformamide	Masaharu Fujitake	Manuscript in prep. Z, E-form
C <sub>5</sub> H <sub>13</sub> NO <sub>2</sub> (C <sub>5</sub> H <sub>11</sub> NO-H <sub>2</sub> O)	N-tert-Butylformamide -water	Masaharu Fujitake	Manuscript in prep. Two conformers
C <sub>5</sub> H <sub>15</sub> NO <sub>3</sub> (C <sub>5</sub> H <sub>11</sub> NO-H <sub>4</sub> O <sub>2</sub> )	N-tert-Butylformamide -(water) <sub>2</sub>	Masaharu Fujitake	Manuscript in prep.
C <sub>6</sub> H <sub>15</sub> NO <sub>2</sub> (C <sub>5</sub> H <sub>11</sub> NO-CH <sub>3</sub> OH)	N-tert-Butylformamide -methanol	Masaharu Fujitake	Manuscript in prep. Two conformers
C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> (C <sub>5</sub> H <sub>11</sub> NO-HCONH <sub>2</sub> )	N-tert-Butylformamide -formamide	Masaharu Fujitake	Spectrum assigned. formamide- <sup>15</sup> N
C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub> (C <sub>4</sub> H <sub>9</sub> NO-H <sub>2</sub> O)	N,N-Dimethylacetamide -water	Masaharu Fujitake	Spectrum assigned. V <sub>3</sub> of 3 methyl tops
C <sub>4</sub> H <sub>10</sub> O <sub>4</sub> (C <sub>4</sub> H <sub>8</sub> O <sub>3</sub> -H <sub>2</sub> O)	Methyl lactate-water	Masaharu Fujitake	Manuscript in prep. Three conformers

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



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>3</sub> H <sub>8</sub> DNO <sub>2</sub> (CH <sub>3</sub> CONHCH <sub>3</sub> -HOD)	N-methylacetamide -(HOD)water	Masaharu Fujitake	Spectrum assigned.
C <sub>3</sub> H <sub>10</sub> O <sub>5</sub> (C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> -(H <sub>2</sub> O) <sub>2</sub> )	Methyl glycolate-(water) <sub>2</sub>	Masaharu Fujitake	Spectrum assigned.
C <sub>4</sub> H <sub>10</sub> O <sub>4</sub> (C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> -CH <sub>3</sub> OH)	Methyl glycolate-methanol	Masaharu Fujitake	Spectrum assigned.
C <sub>4</sub> H <sub>11</sub> NO (NH <sub>2</sub> CH <sub>2</sub> C(CH <sub>3</sub> ) <sub>2</sub> OH)	1-Amino-2-methyl-2-propanol	Masaharu Fujitake	Spectrum assigned.
C <sub>4</sub> H <sub>13</sub> NO <sub>2</sub> (NH <sub>2</sub> CH <sub>2</sub> C(CH <sub>3</sub> ) <sub>2</sub> OH-H <sub>2</sub> O)	1-Amino-2-methyl-2-propanol -water	Masaharu Fujitake	Spectrum assigned. Two conformers
C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> (HCONH <sub>2</sub> -(CH <sub>2</sub> ) <sub>3</sub> O)	Formamide-trimethylene oxide	Masaharu Fujitake	Spectrum assigned.
C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> (HCONH <sub>2</sub> -HCONHCH <sub>3</sub> )	Formamide-N-methylformamide	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 <sub>2</sub> H <sub>3</sub> F <sub>5</sub> O (CF <sub>3</sub> CF <sub>2</sub> H-H <sub>2</sub> O)	pentafluoroethane-water complex	Q. Gou, G. Feng, W. Caminati, <sup>1</sup> J.-U. Grabow, <sup>2</sup> A. Lesarri <sup>3</sup>	Manu. Ready
C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O (CF <sub>3</sub> H-H <sub>2</sub> CO)	Trifluoromethane-formaldehyde complex	Q. Gou <sup>1,3,4</sup>	1 conformer, 4 states
C <sub>2</sub> H <sub>3</sub> F <sub>4</sub> NS <sub>2</sub> (C <sub>2</sub> S <sub>2</sub> F <sub>4</sub> -NH <sub>3</sub> )	Tetrafluoro-1,3-dithietane-ammonia complex	X. Li	Manuscript in preparation; Spectra assigned, <sup>34</sup> S, <sup>13</sup> C and <sup>15</sup> N isotopes, internal rotation
C <sub>2</sub> H <sub>3</sub> F <sub>2</sub> NO (CH <sub>2</sub> F <sub>2</sub> -H <sub>2</sub> NCHO)	CH <sub>2</sub> F <sub>2</sub> -Formamide	T. Lu, J. Lei	Spectra assigned, 1 conformer
C <sub>3</sub> H <sub>3</sub> ClF <sub>4</sub> S <sub>2</sub> (C <sub>2</sub> F <sub>4</sub> S <sub>2</sub> -CH <sub>3</sub> Cl)	Tetrafluoro-1,3-dithietane-CH <sub>3</sub> Cl	T. Lu, J. Lei	Spectra assigned, 1 conformer, <sup>37</sup> Cl isotope, internal rotation of -CH <sub>3</sub> group
C <sub>3</sub> H <sub>4</sub> O <sub>4</sub> (C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> -H <sub>2</sub> O)	Vinylene carbonate-water	J. Chen, T. Lu	Spectra assigned
C <sub>3</sub> H <sub>3</sub> NOS (C <sub>3</sub> H <sub>3</sub> NS-H <sub>2</sub> O)	Thiazole-H <sub>2</sub> O complex	W. Li, J. Chen	Spectra assigned, one conformer, <sup>13</sup> C, <sup>15</sup> N, <sup>34</sup> S, H <sub>2</sub> <sup>18</sup> O, D <sub>2</sub> O, DOH, HOD isotopologues, manuscript submitted.
C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> (C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> -H <sub>2</sub> O)	3-oxetanone-water	J. Chen, T. Lu	Spectra assigned, manuscript in preparation
C <sub>3</sub> H <sub>8</sub> OS (CH <sub>3</sub> SCH <sub>3</sub> -H <sub>2</sub> CO)	Dimethyl sulfide-formaldehyde complex	J. Zhang, S. Gao	Spectra assigned, one conformer

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>2</sub> F <sub>8</sub> O (C <sub>4</sub> F <sub>8</sub> -H <sub>2</sub> O)	octafluorocyclobutane-water	J. Chen <sup>3,8</sup>	Spectra assigned, one conformer, O <sup>18</sup> , D <sub>2</sub> O, DOH, tunneling splitting, four states,
C <sub>4</sub> H <sub>3</sub> F <sub>3</sub> O <sub>2</sub>	2-(Trifluoromethyl)acrylic acid	M. Li, W. Li, Y. Zheng	Spectra assigned, two conformers
C <sub>4</sub> H <sub>3</sub> F <sub>8</sub> N (C <sub>4</sub> F <sub>8</sub> -NH <sub>3</sub> )	octafluorocyclobutane-ammonia	J. Chen	One conformer, tunneling splitting, four states, two of them were assigned
C <sub>4</sub> H <sub>4</sub> F <sub>8</sub> O <sub>2</sub> (C <sub>4</sub> F <sub>8</sub> -2H <sub>2</sub> O)	Octafluorocyclobutane-water trimer	J. Chen, T. Lu, S. Blanco, <sup>3</sup> Z. Kisiel <sup>8</sup>	Spectra assigned, manuscript in preparation
C <sub>4</sub> H <sub>4</sub> F <sub>4</sub> O <sub>4</sub> (CF <sub>2</sub> HCOOH) <sub>2</sub>	$\alpha,\alpha$ -F <sub>2</sub> -acetic acid dimer	Q. Gou <sup>1</sup>	4 states, proton tunneling
C <sub>4</sub> H <sub>5</sub> NOS (C <sub>3</sub> H <sub>3</sub> NS-H <sub>2</sub> CO)	Thiazole-formaldehyde complex	W. Li, W. Cheng	Spectra assigned, three conformers, <sup>13</sup> C, <sup>15</sup> N, <sup>34</sup> S, <sup>18</sup> O isotopologues for one conformer, internal rotation of HCHO group for two conformers
C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub> S	ethoxycarbonyl isothiocyanate	Y.G. Xu, W. Li, J. Zhang	Spectra assigned, two conformers, <sup>13</sup> C, <sup>15</sup> N, <sup>34</sup> S isotopologues
C <sub>4</sub> H <sub>5</sub> F <sub>3</sub> O <sub>3</sub> (C <sub>4</sub> H <sub>3</sub> O <sub>2</sub> F <sub>3</sub> -H <sub>2</sub> O)	2-(Trifluoromethyl)acrylic acid-Water complex	M. Li, W. Li, Y. Zheng	Spectra assigned, two conformers, O <sup>18</sup> isotopologues
C <sub>4</sub> H <sub>5</sub> F <sub>3</sub> O <sub>2</sub> (CH <sub>3</sub> COCF <sub>3</sub> -H <sub>2</sub> CO)	1,1,1-Trifluoroacetone-formaldehyde	Y. Jin, J.-U. Grabow, <sup>2</sup> A. Lesarri <sup>3</sup>	Spectra assigned, manuscript in preparation
C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> (C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> -H <sub>2</sub> CO)	3-oxetanone-formaldehyde	J. Chen, T. Lu	Spectra assigned, tunneling splitting, manuscript in preparation
C <sub>4</sub> H <sub>7</sub> NS (CH <sub>3</sub> ) <sub>2</sub> CHNCS	isopropylisothiocyanate	Y.G. Xu, W. Li, J. Zhang	Spectra assigned, one conformer, <sup>13</sup> C, <sup>15</sup> N, <sup>34</sup> S isotopologues
C <sub>4</sub> H <sub>9</sub> NOS (CH <sub>3</sub> ) <sub>2</sub> CHNCS-H <sub>2</sub> O)	Isopropylisothiocyanate-water	Y.G. Xu, W. Li, J. Zhang	Spectra assigned, one conformer, tunneling splitting.
C <sub>4</sub> H <sub>8</sub> O (HOCH <sub>2</sub> C=CH <sub>2</sub> CH <sub>3</sub> )	Methacryl alcohol	J. Lei, Y. Jin	Spectra assigned, 2 conformers, <sup>13</sup> C isotopologues, internal rotation of -CH <sub>3</sub> and OH
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	4-hydroxy-2-butanone	M. Li, T. Lu	Manuscript in preparation, spectra assigned, one conformer, <sup>13</sup> C isotopologues, internal rotation of -CH <sub>3</sub> group

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>8</sub> S <sub>2</sub> (CH <sub>2</sub> CHCH <sub>2</sub> SSCH <sub>3</sub> )	Allyl methyl disulfide	X. Li, J.-U. Grabow <sup>2</sup>	Spectra assigned, 2 conformers
C <sub>4</sub> H <sub>8</sub> F <sub>6</sub> (CH <sub>2</sub> F <sub>2</sub> ) <sub>2</sub> -CH <sub>3</sub> CHF <sub>2</sub> )	(CH <sub>2</sub> F <sub>2</sub> ) <sub>2</sub> -CH <sub>3</sub> CHF <sub>2</sub> trimer	T. Lu, J. Chen	Manuscript in preparation, 2 conformers, all the <sup>13</sup> C isotopes for the most stable conformer
C <sub>4</sub> H <sub>8</sub> O <sub>3</sub> (CH <sub>3</sub> OCOCH <sub>2</sub> COCH <sub>3</sub> )	Methyl methoxyacetate	J. Lei	Spectra assigned, one conformer, internal rotation of -CH <sub>3</sub>
C <sub>4</sub> H <sub>9</sub> NOS (C <sub>4</sub> H <sub>7</sub> NS-H <sub>2</sub> O)	isopropylisothiocyanate-water complex	Y.G. Xu, W. Li, J. Zhang	Spectra assigned, one conformer, internal rotation of H <sub>2</sub> O
C <sub>4</sub> H <sub>10</sub> OS <sub>2</sub> (CH <sub>2</sub> CHCH <sub>2</sub> SSCH <sub>3</sub> -H <sub>2</sub> O)	Allyl methyl disulfide-H <sub>2</sub> O complex	X. Li, J. Chen, J.-U. Grabow <sup>2</sup>	Spectra assigned, 1 conformer
C <sub>4</sub> H <sub>10</sub> ArS <sub>2</sub> (CH <sub>3</sub> CH <sub>2</sub> S <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> -Ar)	diethyl disulfide-Ar complex	T. Lu, D. A. Obenchain <sup>2</sup>	Manuscript in preparation, 1 conformer
C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> (C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> -H <sub>2</sub> O)	4-hydroxy-2-butanone-Water complex	M. Li, T. Lu	Manuscript in preparation, spectra assigned, one conformer, O <sup>18</sup> , D <sub>2</sub> O, DOH, HOD isotopologues, internal rotation of -CH <sub>3</sub> group
C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> (C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> -H <sub>2</sub> O)	Acetoin monomer, Acetoin-H <sub>2</sub> O	Y. Zheng, T. Lu, W. Cheng, W. Liu	Spectra assigned, 1 conformer, <sup>13</sup> C, OD, C= <sup>18</sup> O, <sup>18</sup> O, DOH, OD-D <sub>2</sub> O isotopes, internal rotation of CH <sub>3</sub>
C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> (CH(OCH <sub>3</sub> ) <sub>3</sub> )	trimethoxymethane	G. Feng <sup>1,5</sup>	3 conformers assigned
C <sub>4</sub> H <sub>12</sub> OS (CH <sub>3</sub> CH <sub>2</sub> OH-CH <sub>3</sub> CH <sub>2</sub> SH)	ethanol-ethanethiol	J. Yan, J. Zhang, X. Li, A. Lesarri <sup>3</sup>	Spectrum assigned, one conformer
C <sub>4</sub> H <sub>12</sub> OS <sub>2</sub> (CH <sub>3</sub> CH <sub>2</sub> S <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> -H <sub>2</sub> O)	diethyl disulfide-water complex	X. Li, J.-U. Grabow <sup>2</sup>	Manuscript in preparation, one conformer, <sup>18</sup> O, D <sub>2</sub> O, DOH, HOD, <sup>34</sup> S isotopes
C <sub>4</sub> H <sub>12</sub> S <sub>2</sub> (CH <sub>3</sub> CH <sub>2</sub> SH-CH <sub>3</sub> CH <sub>2</sub> SH)	ethanethiol-ethanethiol	J. Zhang, X. Li, A. Lesarri <sup>3</sup>	Spectrum assigned, one conformer, tunneling splitting
C <sub>5</sub> HF <sub>4</sub> N (2,3,4,6-C <sub>6</sub> HF)	2,3,4,6-Tetrafluoropyridine	J. Wang	Manuscript in preparation, <sup>13</sup> C and <sup>15</sup> N isotopologues
C <sub>5</sub> H <sub>4</sub> F <sub>3</sub> NO (C <sub>5</sub> H <sub>2</sub> F <sub>3</sub> N-H <sub>2</sub> O)	2,3,6-Trifluoropyridine-water complex	J. Wang <sup>1</sup>	Manuscript in preparation, <sup>18</sup> O, D <sub>2</sub> O, DOH, HOD isotopes

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>5</sub> H <sub>4</sub> ClF <sub>3</sub> O (furan-CF <sub>3</sub> Cl)	furan-CF <sub>3</sub> Cl	Y. Zheng, W. Cheng, W. Liu	Spectra assigned, 2 conformers, <sup>37</sup> Cl, <sup>13</sup> C isotopes, Manuscript in preparation
C <sub>5</sub> H <sub>4</sub> O <sub>3</sub> (C <sub>4</sub> H <sub>4</sub> O-CO <sub>2</sub> )	furan-CO <sub>2</sub>	J. Lei	Spectra assigned, one conformer,
C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub> (C <sub>4</sub> H <sub>5</sub> N-CO <sub>2</sub> )	pyrrole-CO <sub>2</sub> complex	W. Cheng, W. Liu, Y. Zheng	Spectra assigned, one conformer, <sup>15</sup> N, <sup>13</sup> C isotopologues
C <sub>5</sub> H <sub>5</sub> F <sub>2</sub> NO (C <sub>5</sub> H <sub>3</sub> F <sub>2</sub> N-H <sub>2</sub> O)	2,3-difluoropyridine-water complex	J. Wang, S. Melandri <sup>1</sup>	Manuscript in preparation <sup>18</sup> O, D <sub>2</sub> O, DOH, HOD isotopes
C <sub>5</sub> H <sub>5</sub> F <sub>2</sub> NO (C <sub>5</sub> H <sub>3</sub> F <sub>2</sub> N-H <sub>2</sub> O)	2,6-difluoropyridine-water complex	J. Wang, S. Melandri <sup>1</sup>	Manuscript in preparation <sup>18</sup> O, D <sub>2</sub> O, DOH, HOD isotopes
C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub> (C <sub>4</sub> H <sub>9</sub> N-CO <sub>2</sub> )	pyrrolidine-CO <sub>2</sub> complex	W. Cheng, J. Wang	Spectra assigned, two conformers
C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub> (C <sub>4</sub> H <sub>9</sub> ON-CO <sub>2</sub> )	morpholine-CO <sub>2</sub> complex	W. Cheng, J. Zhang	Manuscript in preparation, two conformers
C <sub>5</sub> H <sub>9</sub> F <sub>4</sub> NS <sub>2</sub> (C <sub>3</sub> H <sub>9</sub> N-C <sub>2</sub> S <sub>2</sub> F <sub>4</sub> )	isopropylamine-C <sub>2</sub> S <sub>2</sub> F <sub>4</sub> complex	Y. Jin	Spectra assigned, two conformers, manuscript in preparation.
C <sub>5</sub> H <sub>10</sub> F <sub>6</sub> (CH <sub>2</sub> F <sub>2</sub> -(CH <sub>3</sub> CHF <sub>2</sub> ) <sub>2</sub> )	CH <sub>2</sub> F <sub>2</sub> -(CH <sub>3</sub> CHF <sub>2</sub> ) <sub>2</sub> trimer	T. Lu, J. Chen	Manuscript in preparation, 2 conformers, all the <sup>13</sup> C isotopes for the most stable conformer
C <sub>5</sub> H <sub>12</sub> OS <sub>2</sub> (CH <sub>3</sub> CH <sub>2</sub> S <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> -HCHO)	Diethyl Disulfide-H <sub>2</sub> CO complex	T. Lu, J. Zhang, X. Li, D. A. Obenchain <sup>2</sup> , S. Herbers <sup>2</sup>	Manuscript in preparation, 1 conformer
C <sub>5</sub> H <sub>13</sub> NOS <sub>2</sub> (CH <sub>3</sub> CH <sub>2</sub> S <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> - HCONH <sub>2</sub> )	Diethyl Disulfide-HCONH <sub>2</sub> complex	T. Lu, J. Zhang, X. Li, D. A. Obenchain <sup>2</sup> , S. Herbers <sup>2</sup>	Manuscript in preparation, 1 conformer
C <sub>6</sub> H <sub>2</sub> F <sub>5</sub> N	Pentafluoroaniline	S. Gao	Spectra assigned, one conformer
C <sub>6</sub> H <sub>3</sub> FN	2-Fluoro-4-methylpyridine	S. Gao	Journal of Molecular Structure accepted
C <sub>6</sub> H <sub>5</sub> ClF <sub>3</sub> N (C <sub>6</sub> H <sub>5</sub> N-CClF <sub>3</sub> )	pyridine- trifluorochloromethane complex	Q. Gou <sup>1</sup>	Manuscript submitted

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>5</sub> FNO (C <sub>6</sub> H <sub>3</sub> NF-H <sub>2</sub> O)	2-Fluoro-4-methylpyridine-water complex	S. Gao	Spectra assigned, 1 conformer
C <sub>6</sub> H <sub>7</sub> NO	2-methoxypyridine	W. Cheng, Y. Zheng, J.-U. Grabow <sup>2</sup>	Accepted <i>Spectrochim. Acta Part A</i> .
C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	3-methylcyclopentane-1,2-dione	J. Wang S. Herbers <sup>2</sup>	Manuscript in preparation, one conformer, internal rotation of -CH <sub>3</sub>
C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> (C <sub>5</sub> H <sub>8</sub> -CO <sub>2</sub> )	cyclopentene-carbon dioxide	J. Wang, H. Wang, X. Wang S. Herbers <sup>2</sup>	Manuscript in preparation, one conformer, all <sup>13</sup> C mono-isotopologues
C <sub>6</sub> H <sub>8</sub> O <sub>4</sub> (C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> ) <sub>2</sub>	3-oxetanone homodimer	J. Chen, T. Lu	Spectra assigned, manuscript in preparation
C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub> (C <sub>6</sub> H <sub>7</sub> ON-H <sub>2</sub> O)	2-methoxypyridine-water complex	W. Cheng, Y. Zheng, J.-U. Grabow <sup>2</sup>	Accepted <i>Spectrochim. Acta Part A</i> .
C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> (C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> -H <sub>2</sub> O)	3-methylcyclopentane-1,2-dione -water	J. Wang, S. Herbers <sup>2</sup>	Manuscript in preparation, one conformer, internal rotation of -CH <sub>3</sub>
C <sub>6</sub> H <sub>12</sub> F <sub>6</sub> (CH <sub>3</sub> CHF <sub>2</sub> ) <sub>3</sub>	(CH <sub>3</sub> CHF <sub>2</sub> ) <sub>3</sub> trimer	T. Lu, J. Chen	Manuscript in preparation, 2 conformers, all the <sup>13</sup> C isotopes for the observed conformers
C <sub>7</sub> HF <sub>5</sub> O	Pentafluorobenzaldehyde	J. Wang, X. Li, H. Wang, X. Wang	Spectra assigned, one conformer All isotopologues
C <sub>7</sub> H <sub>3</sub> F <sub>5</sub> (C <sub>6</sub> F <sub>5</sub> OCF <sub>3</sub> )	pentafluoroanisole	X. Li	Spectra assigned, 1 conformer
C <sub>7</sub> H <sub>3</sub> F <sub>5</sub> O <sub>2</sub> (C <sub>7</sub> HOF <sub>5</sub> -H <sub>2</sub> O)	Pentafluorobenzaldehyde-water	J. Wang, X. Li, H. Wang, X. Wang	Spectra assigned, one conformer
C <sub>7</sub> H <sub>5</sub> N	2-Ethynylpyridine	S. Gao, X. Li	Spectra assigned, one conformer
C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> (C <sub>6</sub> H <sub>6</sub> -CO <sub>2</sub> )	phenol-CO <sub>2</sub> complex	H. Wang, J. Wang	Spectra assigned, 1 conformer
C <sub>7</sub> H <sub>7</sub> NO (C <sub>7</sub> H <sub>5</sub> N-H <sub>2</sub> O)	2-Ethynylpyridine-H <sub>2</sub> O complex	S. Gao, X. Li	Spectra assigned, one conformer, O <sup>18</sup> , D <sub>2</sub> O, DOH, HOD

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub> (C <sub>6</sub> H <sub>7</sub> ON-CO <sub>2</sub> )	2-methoxypyridine-CO <sub>2</sub> complex	W. Cheng, Y. Zheng	Spectra assigned, one conformer
C <sub>7</sub> H <sub>7</sub> F <sub>2</sub> N	3,4-Difluorobenzylamine	S. Gao, X. Wang	Spectra assigned, two conformers
C <sub>7</sub> H <sub>7</sub> F <sub>2</sub> N	2,6-Difluorobenzylamine	S. Gao	Spectra assigned, one conformer
C <sub>7</sub> H <sub>7</sub> F <sub>2</sub> N	2,4-Difluorobenzylamine	S. Gao	Spectra assigned, two conformers, -NH <sub>2</sub> tunneling
C <sub>7</sub> H <sub>8</sub> O <sub>4</sub> (C <sub>5</sub> H <sub>8</sub> -CO <sub>2</sub> -CO <sub>2</sub> )	cyclopentene-(carbon dioxide) <sub>2</sub>	J. Wang S. Herbers <sup>2</sup>	Manuscript in preparation, one conformer
C <sub>7</sub> H <sub>8</sub> FN	4-fluorobenzylamine	S. Gao, X. Wang	Spectra assigned, one conformer
C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	Cyclohexanecarboxylic acid	T. Lu, A. S. Hazrah, <sup>7</sup> F. Xie <sup>7</sup>	Spectra assigned, one conformer
C <sub>7</sub> H <sub>14</sub> O <sub>3</sub> (C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> -H <sub>2</sub> O)	Cyclohexanecarboxylic acid-H <sub>2</sub> O	T. Lu, A. S. Hazrah, <sup>7</sup> F. Xie <sup>7</sup>	Spectra assigned, one conformer
C <sub>5</sub> H <sub>11</sub> N	2-Methylpyrrolidine	T. Lu, A. S. Hazrah <sup>7</sup>	Spectra assigned, internal rotation of -CH <sub>3</sub> group
C <sub>5</sub> H <sub>13</sub> NO (C <sub>5</sub> H <sub>11</sub> N-H <sub>2</sub> O)	2-Methylpyrrolidine-H <sub>2</sub> O	T. Lu, A. S. Hazrah <sup>7</sup>	Spectra assigned, 1 conformer, internal rotation of -CH <sub>3</sub> group
C <sub>7</sub> H <sub>14</sub> S	cyclohexylmethanethiol	Y. Jin, R. T. Saragi, <sup>3</sup> A. Lesarri <sup>3</sup>	Spectra assigned, 3 conformers
C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub> (C <sub>7</sub> H <sub>5</sub> N-CO <sub>2</sub> )	2-Ethynylpyridine-CO <sub>2</sub> complex	S. Gao, X. Li	Spectra assigned, one conformer
C <sub>8</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> COCF <sub>3</sub> -H <sub>2</sub> O)	2,2,2-trifluoroacetophenone-water complex	J. Lei	Spectra assigned, one conformer Manuscript in preparation
C <sub>8</sub> H <sub>10</sub> O (C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub> -H <sub>2</sub> O)	Styrene-water complex	Y. Zheng, E. Burevschi <sup>6</sup>	Manuscript in preparation, one conformer, O <sup>18</sup> , D <sub>2</sub> O, DOH, tunneling splitting
C <sub>8</sub> H <sub>12</sub> O <sub>2</sub> (C <sub>8</sub> H <sub>10</sub> O-H <sub>2</sub> O)	1-phenylethanol monomer, 1-phenylethanol-H <sub>2</sub> O	Y. Zheng, W. Cheng	manuscript in preparation, 1 conformer, <sup>18</sup> O, DOH isotopes, tunneling splitting,
C <sub>8</sub> H <sub>16</sub> O	Cyclohexylethanol	Y. Jin, R. T. Saragi, <sup>3</sup> A. Lesarri <sup>3</sup>	Spectra assigned, 2 conformers

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>9</sub> H <sub>8</sub> O <sub>3</sub> (C <sub>8</sub> H <sub>8</sub> O-CO <sub>2</sub> )	Acetophenone-Carbon dioxide complex	M. Li, J. Lei	One conformer, accepted <i>Spectrochim. Acta Part A</i>
C <sub>9</sub> H <sub>10</sub> O	Isochroman	X. Wang, S. Gao, J. Wang	Spectra assigned, one conformer, <sup>13</sup> C isotopologues
C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> (C <sub>8</sub> H <sub>6</sub> O-H <sub>2</sub> CO)	2,3-Benzofuran-formaldehyde complex	X. Li, Y. Zheng, C. Puzzarini <sup>1</sup> , J.-U. Grabow <sup>2</sup>	Spectra assigned, 1 conformer, manuscript in preparation.
C <sub>9</sub> H <sub>18</sub> O <sub>3</sub> (C <sub>9</sub> H <sub>16</sub> O <sub>2</sub> -H <sub>2</sub> O)	1,7-dioxaspiro[5.5]undecane-water complex	Y.G. Xu, W. Li, J. Zhang	Spectra assigned, one conformer
C <sub>14</sub> H <sub>28</sub> S <sub>2</sub> (C <sub>7</sub> H <sub>14</sub> S) <sub>2</sub>	Cyclohexylmethanethiol dimer	Y. Jin, R. T. Saragi, <sup>3</sup> A. Lesarri <sup>3</sup>	Spectra assigned, 1 conformer
C <sub>16</sub> H <sub>32</sub> O <sub>2</sub> (C <sub>8</sub> H <sub>16</sub> O) <sub>2</sub>	Cyclohexylethanol dimer	Y. Jin, R. T. Saragi, <sup>3</sup> A. Lesarri <sup>3</sup>	Spectra assigned, 1 conformer
C <sub>8</sub> H <sub>6</sub> ArO (C <sub>8</sub> H <sub>6</sub> O-Ar)	Benzofuran-Ar	J. Zhang	Spectra assigned, 1 conformer
C <sub>8</sub> H <sub>6</sub> KrO (C <sub>8</sub> H <sub>6</sub> O-Kr)	Benzofuran-Kr	J. Zhang	Spectra assigned, 1 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 <sup>g</sup> B. M. Giuliano <sup>g</sup>	v = 1, I nq-hfs in progress
BaF	barium fluoride	R. J. Mawhorter <sup>l</sup>	isotopologues, fs/hfs measurement in progress
CBr <sub>2</sub> F <sub>2</sub>	dibromo- Difluoromethane	D. A. Obenchain J. Signore <sup>d</sup>	2x Br nq-hfs, cd in progress
CHI <sub>3</sub>	triiodomethane	P. Buschmann K. Lengsfeld	I nq-hfs
CH <sub>5</sub> NO <sub>2</sub>	formic acid ... ammonia	F. Lovas <sup>a</sup> G. T. Fraser <sup>a</sup> R. D. Suenram <sup>f</sup>	lam, N nq-hfs, conformation spectrum assigned
COSXe	carbonyl sulfide ... xenon	S. Herbers D. Wachsmuth D. A. Obenchain P. Kraus	re-structure spectra assigned in press <i>Phys. Chem. Chem. Phys.</i>
C <sub>2</sub> H <sub>3</sub> F <sub>5</sub> O	pentafluoroethane ... water	G. Feng <sup>b</sup> Q. Gou <sup>b</sup> W. Caminati <sup>g</sup> A. Lesarri <sup>c</sup>	lam, structure ms completed
C <sub>2</sub> H <sub>3</sub> NO <sub>3</sub>	formamide carbondioxide	S. Gao <sup>b</sup> D. A. Obenchain J. Lei <sup>b</sup> S. Herbers	N nq-hfs, cd, conformation <i>Phys.Chem.Chem.Phys.</i> 21, 7026(2019)
C <sub>2</sub> H <sub>2</sub> F <sub>4</sub> OS <sub>2</sub>	2,2,4,4-tetrafluoro- 1,3-dithiethane ... water	Y. Jin <sup>b</sup> X. Li <sup>b</sup> W. Caminati <sup>g</sup>	lam, structure <i>Phys.Chem.Chem.Phys.</i> 21, 15656(2019)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>2</sub> H <sub>5</sub> NO	cis N-methyl-formamide	C. Evans <sup>t</sup> , D. McNaughton <sup>k</sup>	N nq-hfs, cd measurements completed
C <sub>2</sub> H <sub>6</sub> Cl <sub>2</sub> Si	dichloro-dimethylsilane	D. Banser W. Caminati <sup>g</sup> , A. Lesarri <sup>e</sup> E. J. Cocinero <sup>o</sup> M. Schnell	lam, Cl nq-hfs analysis in progress
C <sub>2</sub> H <sub>6</sub> Cl <sub>2</sub> Sn	dichloro-dimethylstannane	P. Ottaviani <sup>g</sup> , M. Schnell	lam, Cl nq-hfs spectrum assigned
C <sub>2</sub> H <sub>6</sub> ArF <sub>2</sub> Ge	difluoro-dimethylgermane ...argon	P. Ottaviani <sup>g</sup> , M. Schnell	lam ms in preparation
C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>2</sub> O	methoxyflurane	A. Vega <sup>e</sup> , E. J. Cocinero <sup>o</sup>	2x Cl nq-hfs, cd, conformations in progress
C <sub>3</sub> H <sub>9</sub> ClGe	chloro-trimethylgermane	M. Schnell J. Fritzsche	<sup>73</sup> Ge nq-hfs, cd analysis in progress
C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O	N,N'-dimethylurea	C. Höhne P. Buschmann	lam, nq-hfs analysis in progress
C <sub>4</sub> H <sub>2</sub> O <sub>3</sub>	succinic anhydride	M. K. Jahn, K. P. R. Nair, D. A. Obenchain, P. Godfrey <sup>k</sup> , D. McNaughton <sup>k</sup> , N. Vogt <sup>v</sup> , J. Demaison <sup>n</sup>	fs, cd, theor. struct. calc. in press <i>Phys. Chem. Chem. Phys.</i>
C <sub>4</sub> H <sub>3</sub> F <sub>3</sub> O <sub>3</sub>	methyl 3,3,3-trifluoropyruvate	K. Lengsfeld P. Buschmann P. Kats S. Herbers D. A. Obenchain S. Genuit C. M. Höhne	lam accepted <i>Z. Phys. Chem.</i>

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>4</sub> BrNO <sub>2</sub>	N-Bromosuccinimide	P. Buschmann D. A. Obenchain K. Lengsfeld S. Genuit	N,Br nq-hfs, cd spectra assigned
C <sub>4</sub> H <sub>4</sub> ClNO <sub>2</sub>	N-Chlorosuccinimide	P. Buschmann D. A. Obenchain K. Lengsfeld S. Genuit	N,Cl nq-hfs, cd spectra assigned
C <sub>4</sub> H <sub>5</sub> F <sub>3</sub> O <sub>2</sub>	1,1,1-Trifluoroacetone ...formaldehyde	Y. Jin <sup>b</sup> A. Lesarri <sup>c</sup>	Spectra assigned ms in preparation
C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub>	succinimide	S. Herbers D. A. Obenchain D. McNaughton <sup>k</sup>	N nq-hfs, cd analysis in progress
C <sub>4</sub> H <sub>5</sub> NO <sub>3</sub>	N-Hydroxysuccinimide	P. Buschmann K. Lengsfeld	N nq-hfs analysis in progress
C <sub>4</sub> H <sub>6</sub> F <sub>4</sub> S <sub>3</sub>	2,2,4,4-tetrafluoro-1,3-dithiethane ... dimethylsulfide	D. A. Obenchain L. Spada <sup>g</sup> M. Juanes <sup>e</sup>	rot. spec., cd, conformation r <sub>s</sub> in progress
C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	vinylacetate	S. Genuit	lam, structure high K <sub>a</sub> analysis in progress
C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	methacrylic acid	S. Herbers P. Kraus	r <sub>e</sub> -structure <i>J. Chem. Phys.</i> 150, 144308(2019)
C <sub>4</sub> H <sub>7</sub> NO	methacrylamide	K. Lengsfeld	lam, s-cis (C <sub>s</sub> ), s-trans(C <sub>1</sub> ) r <sub>s</sub> in progress
C <sub>4</sub> H <sub>7</sub> NO	acetone-cyanohydrin	K. Aydt, M. J. Travers, M. K. Jahn	N nq-hfs, cd assignment completed
C <sub>4</sub> H <sub>8</sub> S <sub>2</sub>	allyl methyl-disulfide	X. Li <sup>b</sup>	Spectra assigned, 2 conformers

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>10</sub> ArS <sub>2</sub>	diethyl disulfide ...argon	T. Lu <sup>b</sup> D. A. Obenchain	rot. spec., cd assignment completed
C <sub>4</sub> H <sub>10</sub> OS <sub>2</sub>	allyl methyl- disulfide ...water	X. Li <sup>b</sup> J. Chen <sup>b</sup>	Spectra assigned, 1 conformer
C <sub>4</sub> H <sub>12</sub> OS <sub>2</sub>	diethyl disulfide ...water	X. Li <sup>b</sup> T. Lu <sup>b</sup> D. A. Obenchain J. Zhang <sup>b</sup> S. Herbers	lam, O <sup>18</sup> , D <sub>2</sub> O, DOH, HOD ms in preparation
C <sub>5</sub> HN	pentadiene nitrile	H. S. P. Müller <sup>j</sup> T. Giesen <sup>w</sup>	N nq-hfs, cd accepted <i>J. Mol. Spectrosc.</i>
C <sub>5</sub> H <sub>4</sub> OS	2-thiophene- carboxaldehyde	W. Li <sup>b</sup> M. Li <sup>b</sup> Y. Jin <sup>b</sup>	rot. spec., cd, 2 conf. <i>J. Chem. Phys.</i> 151, 164307(2019)
C <sub>5</sub> H <sub>4</sub> O <sub>3</sub>	itaconic anhydride	D. A. Obenchain S. Herbers C. Höhne P. Buschmann D. McNaughton <sup>k</sup>	rot. spec., cd analysis in progress
C <sub>5</sub> H <sub>4</sub> OS	2-thiophene- carboxaldehyde ...water	W. Li <sup>b</sup> M. Li <sup>b</sup> Y. Jin <sup>b</sup>	rot. spec., cd, 2 conf....H <sub>2</sub> O <i>J. Chem. Phys.</i> 151, 164307(2019)
C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	acetylacetone	W. Caminati <sup>g</sup> , H. G. Kjaergaard <sup>c</sup>	lam, enolic shape deuterated species in progress
C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	methyl methacrylate	S. Herbers P. Kraus	re-structure <i>J. Chem. Phys.</i> 150, 144308(2019) deuterated species in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>5</sub> H <sub>10</sub> O	cyclopentene ...water	J. Wang L. Spada <sup>g</sup> J. Chen <sup>b</sup> S. Gao <sup>b</sup> S. Alessandrini <sup>x</sup>	lam, conformation <i>Angew. Chem.</i> 131, 14073(2019) <i>Angew. Chem. Int. Ed.</i> 58, 13935(2019)
C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	methyl methacrylate ...water	S. Herbers K. Lengsfeld J. Wang P. Buschmann S. Genuit	lam, conformation assignment in progress
C <sub>5</sub> H <sub>12</sub> OS <sub>2</sub>	diethyl disulfide ...formaldehyde	X. Li <sup>b</sup> T. Lu <sup>b</sup> D. A. Obenchain J. Zhang <sup>b</sup> S. Herbers	lam, O <sup>18</sup> ms in preparation
C <sub>5</sub> H <sub>13</sub> NOS <sub>2</sub>	diethyl disulfide ...formamide	X. Li <sup>b</sup> T. Lu <sup>b</sup> D. A. Obenchain J. Zhang <sup>b</sup> S. Herbers	lam, O <sup>18</sup> ms in preparation
C <sub>5</sub> H <sub>16</sub> SiSn	dimethylsilyl- trimethylstannane	J. T. Hougen <sup>a</sup> , M. Schnell	lam assignment in progress
C <sub>6</sub> H <sub>3</sub> F <sub>3</sub> O	3,4,5-trifluoro- phenol	K.P.R. Nair P. Buschmann D. A. Obenchain	rot. spec., cd, r <sub>s</sub> -structure assignment completed
C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> O	2,3-difluoro - phenol	K.P.R. Nair S. Herbers D. Dewald D. Wachsmuth	rot. spec., cd, r <sub>s</sub> -structure <i>J. Mol. Struct.</i> 1195, 479(2019)
C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> O	2,5-difluoro - phenol	K.P.R. Nair	rot. spec., cd, r <sub>s</sub> -structure spectrum assigned
C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> O	3,4-difluoro - phenol	K.P.R. Nair	rot. spec., cd, r <sub>s</sub> -structure spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> O	3,5-difluoro - phenol	D. Dewald	lam analysis completed
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	2-cyano pyridine	D. Prudenzano, D. Wachsmuth, M. K. Jahn, D. McNaughton <sup>k</sup>	2x N nq-hfs, r <sub>s</sub> -structure ms in preparation
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	3-cyano pyridine	D. Prudenzano, D. Wachsmuth, M. K. Jahn, D. McNaughton <sup>k</sup>	2x N nq-hfs, r <sub>s</sub> -structure ms in preparation
C <sub>6</sub> H <sub>5</sub> BrO	ortho-bromo-phenol	K.P.R. Nair K. Lengsfeld P. Buschmann J. Wang	Br nq-hfs analysis in progress
C <sub>6</sub> H <sub>5</sub> ClO	ortho-chloro-phenol	K.P.R. Nair K. Lengsfeld P. Buschmann J. Wang	Cl nq-hfs analysis in progress
C <sub>6</sub> H <sub>5</sub> ClO	meta-chloro-phenol	P. Buschmann K. Lengsfeld D. Dewald D. Wachsmuth	conformations, Cl nq-hfs accepted <i>J. Mol. Struct.</i>
C <sub>6</sub> H <sub>5</sub> ClO	para-chloro-phenol	P. Buschmann K. Lengsfeld D. Dewald D. Wachsmuth	extended Townes-Daily, Cl nq-hfs accepted <i>J. Mol. Struct.</i>
C <sub>6</sub> H <sub>5</sub> IO	ortho-iodo-phenol	K.P.R. Nair K. Lengsfeld P. Buschmann J. Wang	I nq-hfs analysis in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>7</sub> N	4-picoline	S. Herbers M. K. Jahn D. Wachsmuth J. Matysik <sup>i</sup> V. V. Ilyushin <sup>p</sup> W. Caminati <sup>g</sup>	lam, N nq-hfs analysis in progress
C <sub>6</sub> H <sub>7</sub> NO	2-methoxypyridine	W. Cheng <sup>b</sup> J. Zhang <sup>b</sup>	conformation accepted <i>Spectrochim. Acta A.</i>
C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	cyclopentene ...carbon dioxide	J. Wang S. Herbers	r <sub>s</sub> -structure ms in preparation
C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	3-methylcyclo- pentane-1,2-dione	J. Wang S. Herbers P. Buschmann	lam, structure ms in preparation
C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>	citric acid	C. Höhne P. Buschmann K. Lengsfeld	rot. spec., cd analysis in progress
C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub>	2-methoxypyridine ...water	W. Cheng <sup>b</sup> J. Zheng <sup>b</sup>	conformation accepted <i>Spectrochim. Acta A.</i>
C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>	3-methylcyclo- pentane-1,2-dione ...water	J. Wang S. Herbers P. Buschmann	lam, structure ms in preparation
C <sub>6</sub> H <sub>11</sub> NO	ε-caprolactam	D. Wachsmuth M. Vallejo <sup>e</sup>	pseudo-rot., N nq-hfs spectra assigned
C <sub>6</sub> H <sub>12</sub> O	oxepane	J. Borter, D. Wachsmuth, A. Lesarri <sup>e</sup>	pseudo-rot. spectrum assigned
C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	methyl methacrylate ...methanol	S. Herbers K. Lengsfeld J. Wang P. Buschmann S. Genuit	lam, conformation assignment in progress
C <sub>6</sub> H <sub>13</sub> N	azepane	D. Wachsmuth, M. Vallejo <sup>e</sup>	pseudo-rot., N nq-hfs spectra assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>7</sub> H <sub>5</sub> F <sub>3</sub>	2,4,5-trifluoro-toluene	K. P. R. Nair S. Herbers	lam, r <sub>s</sub> -structure accepted <i>Can. J. Phys.</i>
C <sub>7</sub> H <sub>5</sub> F <sub>3</sub>	2,3,4-trifluoro-toluene	K. P. R. Nair S. Herbers	lam, r <sub>s</sub> -structure accepted <i>Can. J. Phys.</i>
C <sub>7</sub> H <sub>6</sub> F <sub>2</sub>	3,4-difluoro-toluene	K. P. R. Nair S. Herbers	lam, Stark effect, r <sub>s</sub> -structure <i>J. Mol. Spectrosc.</i> 355, 19(2019)
C <sub>7</sub> H <sub>6</sub> ClF	2-Chloro-4-fluoro-toluene	K. P. R. Nair S. Herbers D. A. Obenchain A. Lesarri <sup>e</sup>	lam, nq-hfs ms in preparation
C <sub>7</sub> H <sub>7</sub> Br	ortho-bromo-toluene	K. P. R. Nair S. Herbers, J. Wang, P. Buschmann K. Lengsfeld	lam, Br nq-hfs accepted <i>Phys. Chem. Chem. Phys.</i>
C <sub>7</sub> H <sub>7</sub> Br	meta-bromo-toluene	K. Lengsfeld P. Buschmann H. V. L. Nguyen <sup>m,q</sup>	lam, Br nq-hfs assignment in progress
C <sub>7</sub> H <sub>7</sub> Cl	ortho-chloro-toluene	K. P. R. Nair S. Herbers, J. Wang, P. Buschmann K. Lengsfeld	lam, Cl nq-hfs accepted <i>Phys. Chem. Chem. Phys.</i>
C <sub>7</sub> H <sub>7</sub> Cl	meta-chloro-toluene	K. P. R. Nair S. Herbers, A. Lesarri <sup>e</sup>	lam, Cl nq-hfs <i>J. Mol. Spectrosc.</i> 361, 1(2019)
C <sub>7</sub> H <sub>7</sub> Cl	para-chloro-toluene	K. P. R. Nair V. V. Ilyushin <sup>p</sup>	lam, Cl nq-hfs ms in preparation
C <sub>7</sub> H <sub>7</sub> F	ortho-fluoro-toluene	K. P. R. Nair S. Herbers, J. Wang, P. Buschmann K. Lengsfeld	lam, substituent effects accepted <i>Phys. Chem. Chem. Phys.</i>



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>7</sub> H <sub>7</sub> F	meta-fluoro-toluene	K. P. R. Nair S. Herbers H. V. L. Nguyen <sup>m,q</sup>	lam, r <sub>s</sub> -structure ms in preparation
C <sub>7</sub> H <sub>7</sub> I	ortho-iodo-toluene	K. P. R. Nair S. Herbers J. Wang P. Buschmann K. Lengsfeld	lam, I nq-hfs accepted <i>Phys. Chem. Chem. Phys.</i>
C <sub>7</sub> H <sub>7</sub> N	phenylmethan-imine	A. Melli <sup>g</sup> S. Herbers L. Spada <sup>g</sup> K. Lengsfeld	isomers, N nq-hfs ms in preparation
C <sub>7</sub> H <sub>12</sub>	cycloheptene	D. Wachsmuth	rot. spec., cd, structure spectrum assigned
C <sub>7</sub> H <sub>12</sub> O	cycloheptanone	D. Wachsmuth, M. K. Jahn	pseudo-rot. spectrum assigned
C <sub>8</sub> H <sub>4</sub> N <sub>2</sub>	1,2-dicyano-benzene	E. Locatelli D. Dewald M. K. Jahn	N nq-hfs, cd, structure ms in preparation
C <sub>8</sub> H <sub>4</sub> N <sub>2</sub>	1,3-dicyano-benzene	D. Dewald M. K. Jahn M. Jüstel F. Lovas <sup>a</sup>	N nq-hfs, cd, structure ms in preparation
C <sub>8</sub> H <sub>8</sub> O	para-tolualdehyde	W. Caminati <sup>g</sup> A. Hight-Walker <sup>a</sup> J. T. Hougen <sup>a</sup> I. Kleiner <sup>q</sup> J. Gauß <sup>h</sup> H. Saal	int. rot. potential ab-initio tors. analysis ms in preparation
C <sub>8</sub> H <sub>8</sub> O	acetophenone	J. Lei <sup>b</sup> J. Zhang <sup>b</sup>	conformation <i>Phys.Chem.Chem.Phys.</i> 21, 22888(2019)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	acetophenone ···water	J. Lei <sup>b</sup> J. Zhang <sup>b</sup>	conformation <i>Phys.Chem.Chem.Phys.</i> 21, 22888(2019)
C <sub>8</sub> H <sub>11</sub> N	2-ethylaniline	J. Wang S. Herbers, P. Buschmann K. Lengsfeld	N nq-hfs, cd in press <i>Chin. J. Chem. Phys.</i>
C <sub>8</sub> H <sub>11</sub> N	3-ethylaniline	J. Wang S. Herbers, P. Buschmann K. Lengsfeld	N nq-hfs, cd in press <i>Chin. J. Chem. Phys.</i>
C <sub>8</sub> H <sub>11</sub> N	4-ethylaniline	J. Wang S. Herbers, P. Buschmann K. Lengsfeld	N nq-hfs, cd in press <i>Chin. J. Chem. Phys.</i>
C <sub>8</sub> H <sub>12</sub> N	cyanocycloheptane	D. Wachsmuth A. Lesarri <sup>c</sup>	lam, N nq-hfs, conformation ms in preparation
C <sub>9</sub> H <sub>6</sub> N <sub>2</sub>	3-cyanoindole	K. P. R. Nair P. Buschmann K. Lengsfeld J. Wang S. Herbers D. McNaughton <sup>k</sup> M. Schmitt <sup>r</sup>	r <sub>s</sub> structure, N nq-hfs Spectrum assigned
C <sub>9</sub> H <sub>6</sub> N <sub>2</sub>	4-cyanoindole	K. P. R. Nair P. Buschmann K. Lengsfeld J. Wang S. Herbers D. McNaughton <sup>k</sup> M. Schmitt <sup>r</sup>	r <sub>s</sub> structure, N nq-hfs Spectrum assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>9</sub> H <sub>6</sub> N <sub>2</sub>	5-cyanoindole	K. P. R. Nair P. Buschmann K. Lengsfeld J. Wang S. Herbers D. McNaughton <sup>k</sup> M. Schmitt <sup>f</sup>	r <sub>s</sub> structure, N nq-hfs Spectrum assigned
C <sub>9</sub> H <sub>6</sub> N <sub>2</sub>	6-cyanoindole	K. P. R. Nair P. Buschmann K. Lengsfeld J. Wang S. Herbers D. McNaughton <sup>k</sup> M. Schmitt <sup>f</sup>	r <sub>s</sub> structure, N nq-hfs Spectrum assigned
C <sub>9</sub> H <sub>6</sub> N <sub>2</sub>	7-cyanoindole	K. P. R. Nair P. Buschmann K. Lengsfeld J. Wang S. Herbers D. McNaughton <sup>k</sup> M. Schmitt <sup>f</sup>	r <sub>s</sub> structure, N nq-hfs Spectrum assigned
C <sub>9</sub> H <sub>6</sub> O <sub>2</sub>	coumarin	H. V. L. Nguyen <sup>m,q</sup>	rot. spec., cd, structure accepted <i>ChemPhysChem</i>
C <sub>9</sub> H <sub>7</sub> NO	8-hydroxy-quinoline	D. Wachsmuth, S. Herbers, J. Wang, P. Kraus, D. McNaughton <sup>k</sup>	rot. spec., cd, N nq.hfs r <sub>e</sub> structure heavy atom species assigned ms in preparation
C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	2,3-Benzofuran ...formaldehyde	X. Li Y. Zheng K. Lengsfeld C. Puzzarini <sup>g</sup>	structure spectra assigned
C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	acetophenone ...carbon dioxide	M. Li <sup>b</sup> J. Lei <sup>b</sup>	structure accepted <i>Spectrochim. Acta A.</i>

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>10</sub> H <sub>10</sub> O	4-Phenyl-3-buten-2-on	P. Buschmann A. Sander S. Herbers K. Lengsfeld	lam, s-cis, s-trans assignment completed r <sub>s</sub> in progress
C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>	butamben	M. Vallejo <sup>e</sup> , W. Caminati <sup>g</sup> E. J. Cocinero <sup>o</sup> A. Lesarri <sup>e</sup>	conformation(s), r <sub>s</sub> -structure accepted <i>Chem. Comm.</i>
C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub>	isobutamben	M. Vallejo <sup>e</sup> , W. Caminati <sup>g</sup> E. J. Cocinero <sup>o</sup> A. Lesarri <sup>e</sup>	conformation(s), r <sub>s</sub> -structure accepted <i>Chem. Comm.</i>
ClFLi <sub>2</sub>	dilithium chloride fluoride	R. J. Mawhorter <sup>l</sup>	structure measurement in progress
ClRb	rubidium chloride	R. J. Mawhorter <sup>l</sup>	isotopologues, fs/hfs assignment completed
CsF <sub>2</sub> Li	lithium caesium difluoride	R. J. Mawhorter <sup>l</sup>	structure measurement in progress
CuI	copper iodide	L. Bizzocchi <sup>g</sup> , B. M. Giuliano <sup>g</sup>	nq-hfs, spin-spin coupling, v = 1, in progress
FK	potassium fluoride	R. J. Mawhorter <sup>l</sup>	isotopologues, fs/hfs assignment completed
FPb	lead fluoride	R. J. Mawhorter <sup>l</sup> T. J. Sears <sup>s</sup>	isotopologues, fs/hfs, Zeeman effect v > 0, measurement in progress
FRb	rubidium fluoride	R. J. Mawhorter <sup>l</sup>	isotopologues, fs/hfs assignment completed
FYb	ytterbium fluoride	R. J. Mawhorter <sup>l</sup> , T. C. Steimle <sup>u</sup>	isotopologues, fs/hfs <i>Phys. Rev. A</i> 100, 022516(2019)
F <sub>2</sub> KLi	lithium potassium difluoride	R. J. Mawhorter <sup>l</sup>	structure assignment completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
F <sub>2</sub> LiRb	lithium rubidium difluoride	R. J. Mawhorter <sup>l</sup>	structure measurement in progress
HOYb	ytterbium hydroxide	R. J. Mawhorter <sup>l</sup> , T. C. Steimle <sup>u</sup> N. R. Hutzler <sup>y</sup>	isotopologues, fs/hfs measurement in progress
IK	potassium iodide	R. J. Mawhorter <sup>l</sup>	isotopologues, fs/hfs assignment completed
IRb	rubidium iodide	R. J. Mawhorter <sup>l</sup>	isotopologues, fs/hfs assignment completed

The Hannover FTMW spectrometer control & analysis software is available at:  
<http://www.pci.uni-hannover.de/~lgpca/spectroscopy/ftmw> (temporarily down)  
<https://1drv.ms/u/s!AioD2HdE1Y6jgRVP7VADSexL3pZWw?e=9CXTkm> (temporarily up)

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FORMULA	NAME OF COMPOUND	INVESTIGATOR	PRESENT STAGE OF PROGRESS
C <sub>2</sub> H <sub>6</sub> O (CHD <sub>2</sub> OCH <sub>3</sub> )	dimethyl ether-1,1-d <sub>2</sub>	Richard, <sup>a</sup> Motyienko, <sup>b</sup> Margulès <sup>b</sup>	2 conformers assigned fit in progress
C <sub>2</sub> H <sub>7</sub> P	ethylphosphine		ERHAM analysis for doublets or quartets in vib exc 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 <sub>2</sub> HBrF <sub>4</sub>	2-Bromo-1,1,1,2-tetrafluoroethane	J. Isert <sup>1</sup> , F.E. Marshall <sup>1</sup> , W.C. Bailey <sup>7</sup> , G.S. Grubbs II <sup>1</sup>	<i>J. Mol. Struct.</i> <b>1216</b> (2020) 128277
C <sub>2</sub> H <sub>12</sub> Si <sub>3</sub>	Trisilapentane	Atef Jabri <sup>19</sup> , F. E. Marshall <sup>1</sup> , W. R. N. Tonks <sup>10</sup> , R. E. Brenner <sup>9</sup> , D. J. Gillcrist <sup>1</sup> , C. J. Wurrey <sup>9</sup> , I. Kleiner <sup>19</sup> , G. A. Guirgis <sup>10</sup> , G. S. Grubbs II <sup>1</sup>	<i>J. Phys. Chem. A</i> <b>124</b> (2020) 3825
AgClD <sub>2</sub> AgClDH (D <sub>2</sub> -AgCl and HD-AgCl)	Deuterium-Silver Chloride complex	D. A. Obenchain <sup>2</sup> , G. S. Grubbs II <sup>1</sup> , D. S. Frank, H. M. Pickett <sup>2</sup> , S. E. Novick <sup>2</sup>	Manuscript in Prep.
C <sub>11</sub> H <sub>18</sub> O	Nopol	F. E. Marshall <sup>1</sup> , A. J. Duerden <sup>1</sup> , N. Moon <sup>1</sup> , G. Sedo <sup>8</sup> , G. S. Grubbs II <sup>1</sup>	Manuscript in Prep.
C <sub>3</sub> ClF <sub>6</sub> O	Chloroperfluoroacetone	W.C. Bailey <sup>7</sup> , S.A. Cooke <sup>4</sup> , G.S. Grubbs II <sup>1</sup>	Manuscript in Prep. with C <sub>3</sub> Cl <sub>2</sub> F <sub>4</sub> O
C <sub>3</sub> Cl <sub>2</sub> F <sub>4</sub> O	1,3-dichloro-1,1,3,3- tetrafluoroacetone	W.C. Bailey <sup>7</sup> , S.A. Cooke <sup>4</sup> , G.S. Grubbs II <sup>1</sup>	Manuscript in Prep. with C <sub>3</sub> ClF <sub>6</sub> O
C <sub>3</sub> H <sub>2</sub> ClF <sub>3</sub> O	1-chloro-3,3,3- trifluoroacetone	S. A. Cooke <sup>4</sup> and G. S. Grubbs II <sup>1</sup>	Manuscript in Prep.
CF <sub>2</sub> I <sub>2</sub>	Difluorodiiodomethane	G. S. Grubbs II <sup>1</sup> , S. Novick <sup>2</sup> , S. A. Cooke <sup>4</sup>	Experiments Completed; Assignments in Progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
BaS	Barium Monosulfide	G. S. Grubbs II <sup>1</sup> , C. T. Dewberry <sup>5</sup> , K. C. Etchison <sup>6</sup> , S. A. Cooke <sup>4</sup>	Manuscript in Prep.
C <sub>4</sub> H <sub>6</sub> F <sub>2</sub> Si	1,1-Difluorosilacyclopent-2-ene	T. McFadden <sup>10</sup> , F. E. Marshall <sup>1</sup> , G. Jones <sup>10</sup> , T. Carrigan-Broda <sup>10</sup> , G. Guirgis <sup>10</sup> , J. Laane <sup>18</sup> , G. S. Grubbs II <sup>1</sup>	Submitted: <i>J. Phys Chem A</i>
C <sub>4</sub> H <sub>6</sub> F <sub>2</sub> Si	1,1-Difluorosilacyclopent-3-ene	T. McFadden <sup>10</sup> , F. E. Marshall <sup>1</sup> , A.J. Duerden <sup>1</sup> , G. Jones <sup>10</sup> , T. Carrigan-Broda <sup>10</sup> , G.A. Guirgis <sup>10</sup> , G.S. Grubbs II <sup>1</sup>	Manuscript in Prep.
C <sub>4</sub> H <sub>8</sub> F <sub>2</sub> Si	1,1-Difluorosilacyclopentane	F. Marshall <sup>1</sup> , D. Gillcrist <sup>1</sup> , G. Jones <sup>10</sup> , T. Carrigan-Broda <sup>10</sup> , G. Guirgis <sup>10</sup> , G. Grubbs II <sup>1</sup>	Manuscript in Prep.
C <sub>4</sub> H <sub>8</sub> Si	Silacyclopent-3-ene	F. Marshall <sup>1</sup> , N. Moon <sup>1</sup> , G. Jones <sup>10</sup> , T. Carrigan-Broda <sup>10</sup> , G. Guirgis <sup>10</sup> , G. S. Grubbs II <sup>1</sup>	Manuscript in Prep.
C <sub>5</sub> H <sub>10</sub> ClFSi	1-Fluoro-1-chloromethylsilacyclopentane	F. Marshall <sup>1</sup> , T. McFadden <sup>10</sup> , G. Jones <sup>10</sup> , T. Carrigan-Broda <sup>10</sup> , G. Guirgis <sup>10</sup> , G. S. Grubbs II <sup>1</sup>	Experiments Completed; Assignments in Progress
ClU	Uranium Chloride	A. J. Duerden <sup>1</sup> , N. Moon <sup>1</sup> , G. S. Grubbs II <sup>1</sup>	Experiments in Progress
C <sub>4</sub> H <sub>6</sub> F <sub>3</sub> I	3-iodo-1,1,1-trifluorobutane	J. Isert <sup>1</sup> , F. E. Marshall <sup>1</sup> , G. S. Grubbs II <sup>1</sup>	Manuscript in Prep.
ClCuH <sub>2</sub> (H <sub>2</sub> -CuCl)	Hydrogen-Copper Chloride complex	D. Obenchain <sup>2</sup> , G. S. Grubbs II <sup>1</sup> , H. Pickett <sup>2</sup> , S. Novick <sup>2</sup>	Experiments Completed; Assignments in Progress
C <sub>3</sub> H <sub>5</sub> ClO	Chloroacetone	F. E. Marshall <sup>1</sup> , S. A. Cooke <sup>4</sup> , G.S. Grubbs II <sup>1</sup>	Experiments Completed; Assignments in Progress



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_7F_5O_5$ ( $C_3HF_5O_2-(H_2O)_3$ )	Perfluoropropionic Acid Trihydrate Complex	G. S. Grubbs II <sup>1</sup> , D. A. Obenchain <sup>2</sup> , S. A. Cooke <sup>4</sup> , S. E. Novick <sup>2</sup> , A. Serrato III <sup>3</sup> , W. Lin <sup>3</sup>	Experiments Completed; Assignments in Progress
$H_2O_3$ ( $H_2O-O_2$ )	Water-Oxygen vdW complex	A. J. Duerden <sup>1</sup> , F. E. Marshall <sup>1</sup> , N. Moon <sup>1</sup> , T. D. Persinger <sup>1</sup> , G. S. Grubbs II <sup>1</sup>	Experiments Completed; Assignments in Progress
$C_{10}H_{18}O$	Endo-(-)-Borneol	G. Sedo <sup>8</sup> , A. J. Duerden <sup>1</sup> , N. Moon <sup>1</sup> , G. Grubbs II <sup>1</sup>	Experiments Completed; 1 Conformer Assigned
$C_{14}H_{20}O$	Verbenone-3-butyn-2-ol vdW Complex (chiral tag)	L. Evangelisti <sup>14</sup> , K. Mayer <sup>13</sup> , M. Holdren <sup>13</sup> , T. Smart <sup>13</sup> , C. West <sup>13</sup> , B. Pate <sup>13</sup> , G. Sedo <sup>8</sup> , F. Marshall <sup>1</sup> , G.S. Grubbs II <sup>1</sup>	Assignments in Progress
ClPb	Lead Monochloride	G. S. Grubbs II <sup>1</sup> , S. Norman <sup>1</sup> , R. Dawes <sup>1</sup> , B. E. Long <sup>2</sup> , C. T. Dewberry <sup>5</sup> , S. A. Cooke <sup>4</sup>	Experiments Completed; Assignments in Progress
$CO_3$ ( $CO-O_2$ )	Carbon Monoxide- Oxygen vdW complex	F. E. Marshall <sup>1</sup> , D. J. Gillcrist <sup>1</sup> , N. Moon <sup>1</sup> , T. D. Persinger <sup>1</sup> , G. S. Grubbs II <sup>1</sup>	Experiments in Progress
$ClHO_2$ ( $HCl-O_2$ )	Hydrogen Chloride- Oxygen vdW complex	A. J. Duerden <sup>1</sup> , F. E. Marshall <sup>1</sup> , D. J. Gillcrist <sup>1</sup> , N. Moon <sup>1</sup> , T. D. Persinger <sup>1</sup> , G. S. Grubbs II <sup>1</sup>	Experiments Completed; Assignments in Progress
EXPERIMENTAL	Multiple Antennae Design CP-FTMW (MAD-CP- FTMW)	F. E. Marshall <sup>1</sup> , A. J. Duerden <sup>1</sup> , N. Moon <sup>1</sup> , C. Swanson <sup>1</sup> , J. Isert <sup>1</sup> , G. S. Grubbs II <sup>1</sup>	Submitted: <i>J. Mol. Spectrosc.</i>
EXPERIMENTAL	Low-Cost Balle-Flygare FTMW Experiment	A. J. Duerden <sup>1</sup> , N. Moon <sup>1</sup> , G. S. Grubbs II <sup>1</sup>	Submitted: <i>J. Chem. Ed.</i> with Teaching Lab

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
ANALYSIS/DATABASE	Rotational Spectroscopy Teaching Laboratory	A. J. Duerden <sup>1</sup> , N. Moon <sup>1</sup> , G. S. Grubbs II <sup>1</sup>	Submitted: <i>J. Chem. Ed.</i> With Low-Cost 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 <sub>2</sub> H <sub>3</sub> (H <sub>2</sub> CC <sub>2</sub> H)	Vinyl	K. Tanaka Y. Endo	Proton tunneling P-branch transition was observed by FTMW spectroscopy.
C <sub>2</sub> H <sub>3</sub> (HDC <sub>2</sub> H)	Vinyl	M. Hayashi H. Matsubayashi T. Ichiyama K. Harada K. Tanaka	Pure rotational transitions for the cis-tautomer J. Chem. Phys. <b>151</b> , 184304 (2019)
C <sub>2</sub> D <sub>3</sub> (D <sub>2</sub> CCD)	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 <sub>7</sub> H <sub>6</sub> O <sub>2</sub> (C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> D)	Tropolone	H. Matsumoto	Pure rotational transitions. Manuscript in preparation.
C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> (C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> D)	Tropolone	K. Tanaka Y. Endo	FTMW spectra of tunneling rotation transitions. Manuscript in preparation.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_7H_6O_2$ ( $^{13}C_6H_6O_2$ )	Tropolone	K.Tanaka Y. Endo	Pure rotational and tunneling rotation transitions of $^{13}C$ isotopic substituted species. Manuscript in preparation.
$C_7H_6O_2$ ( $C_6H_6^{16}O^{18}O$ ) ( $C_6H_6^{18}O_2$ )	Tropolone	K.Tanaka Y. Endo	Pure rotational and tunneling rotation transitions of $^{18}O$ isotopic substituted species.
$C_3H_4O_2$	Malonaldehyde	T. Baba K. Tanaka	Proton tunneling spectrum. Collaboration with Dr. K.M.T. Yamada (NIRE).
CHHeN (He-HCN)	Helium-hydrogen cyanide complex	K. Harada K. Tanaka	Millimeterwave spectrum of internal rotation hot band and intermolecular stretching band. Manuscript in preparation.
HHeN (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. Manuscript 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 <sub>3</sub> N (H <sub>2</sub> -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.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH <sub>3</sub> N (H <sub>2</sub> -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 <sub>3</sub> (H <sub>2</sub> -HCl)	Hydrogen-hydrogen chloride complex	M. Ishiguro	Pure rotational spectrum assigned and analyzed.
ClH <sub>3</sub> (H <sub>2</sub> -DCl)	Hydrogen-hydrogen chloride complex	K. Nagata	Pure rotational spectrum observed and analyzed.
FH <sub>3</sub> (H <sub>2</sub> -HF) (H <sub>2</sub> -DF)	Hydrogen-hydrogen fluoride complex	T. Moriyama Y. Iwasaki	Pure rotational spectrum observed.
CHFO <sub>2</sub> (OCO-HF) (OCO-DF)	Carbon dioxide-hydrogen fluoride complex	K. Harada M. Ishiguro C. Whitham	Millimeterwave spectrum of vdw bend band.
H <sub>4</sub> O (H <sub>2</sub> -H <sub>2</sub> O) (H <sub>2</sub> -D <sub>2</sub> O)	Hydrogen-water complex	K. Harada C. Whitham Y. Iwasaki T. Giesen K. Tanaka	Pure rotational millimeterwave spectrum observed. Manuscript in preparation.
C <sub>2</sub> H <sub>2</sub> N <sub>2</sub> (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 <sub>2</sub> H <sub>2</sub> N (CH <sub>2</sub> CN)	Cyanomethyl radical	M. J. Tsuchiya	Spectrum in excited vibrational states observed.
Cl <sub>2</sub> Sn (SnCl <sub>2</sub> )	Tin dichloride	K. Uemura	Spectrum assigned.
FGe <sup>+</sup> (GeF <sup>+</sup> )	Germanium fluoride ion	K. Tanaka	In progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_6$	Cyclopropane	K. Tanaka	Centrifugal distortion induced transitions.
$C_3H_4$	Allene	K. Tanaka	Vibrationally induced transitions. Manuscript in preparation.
$F_3OP$ ( $POF_3$ )	Phosphoryl fluoride	K. Someya	LMDR in excited states in progress.
$F_3HSi$ ( $HSiF_3$ ) ( $DSiF_3$ )	Trifluorosilane	K. Harada	LMDR Manuscript in preparation.
$CH_3F$ ( $CH_3F$ ) ( $CD_3F$ )	Methyl fluoride	K. Harada	LMDR Manuscript in preparation.
$CH_3I$	Methyl iodide	K. Harada	LMDR in progress.
$C_2HF$ ( $HCCF$ )	Fluoroacetylene	Y. Nakahara	LMDR in progress.
$C_2H_3N$ ( $CH_3CN$ )	Methyl cyanide	T. Oyama	LMDR in progress.
$C_2H_3N$ ( $CH_3NC$ )	Methyl isocyanide	T. Oyama	LMDR Manuscript in preparation.
$C_3HN$ ( $DCCCN$ )	Cyanoacetylene	K. Tanaka	LMDR in progress.
$CFN$ ( $FCN$ )	Cyanogen fluoride	S. Matsuba	LMDR in progress.
$ClF_5S$ ( $SClF_5$ )	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 <sub>6</sub> H <sub>10</sub> S	7-Thiabicyclo [2.2.1]heptane	K. Irie	Work in progress.
HNO	Nitroxyl	K. Takagi <sup>b</sup> S. Saito <sup>c</sup>	Manuscript in preparation.
CISO[CISO]	CISO radical	S. Saito <sup>c</sup>	Work almost completed.
CH <sub>3</sub> O <sub>2</sub> [CH <sub>3</sub> OO]	Methyl peroxide	K. Katoh <sup>d</sup> Y. Endo <sup>d</sup> E. Hirota	Manuscript in preparation.
C <sub>4</sub> H <sub>6</sub> D <sub>2</sub>	Cyclobutane-1,2-d <sub>2</sub>	E. Hirota	<i>cis, trans</i> , work completed.
C <sub>4</sub> H <sub>4</sub> D <sub>4</sub>	Cyclobutane-1,1,3,3,-d <sub>4</sub>	E. Hirota	Work completed.
KO	Potassium monoxide	C. Yamada	<sup>2</sup> Π, <sup>2</sup> Σ <sup>+</sup> , work almost completed.
BH <sub>4</sub> N	Aminoborane	W. Lewis-Bevan	Work almost completed.
BH <sub>4</sub> Li	Lithium tetrahydroborate	Y. Kawashima <sup>a</sup>	Excited vibrational states, work in progress.
BH <sub>4</sub> K	Potassium tetrahydroborate	Y. Kawashima <sup>a</sup>	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 <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O [N <sub>2</sub> -(CH <sub>3</sub> ) <sub>2</sub> O]	Dinitrogen-dimethyl ether	Y. Kawashima <sup>a</sup> E. Hirota	Spectra assigned for N <sub>2</sub> , N <sup>15</sup> N, <sup>15</sup> N <sub>2</sub> species.
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> [NH <sub>2</sub> COCH <sub>2</sub> CONH <sub>2</sub> ]	Malonamide	T. Usami <sup>a</sup> Y. Kawashima <sup>a</sup> R. D. Suenram <sup>c</sup> E. Hirota	Manuscript prepared.
C <sub>3</sub> H <sub>6</sub> O [CH <sub>3</sub> CH(O)CH <sub>2</sub> ]	Propylene oxide	E. Hirota Y. Kawashima <sup>a</sup>	Work completed.
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S [CO <sub>2</sub> -(CH <sub>3</sub> ) <sub>2</sub> S]	Carbon dioxide-dimethyl-sulfide	S. Iwano <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Work in progress, two states assigned.
C <sub>3</sub> H <sub>7</sub> NO [HCONHCH <sub>2</sub> CH <sub>3</sub> ]	<i>N</i> -Ethylformamide	K. Ohba <sup>a</sup> T. Usami <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Second conformer assigned.
C <sub>3</sub> H <sub>8</sub> OS [OHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> SH]	3-Mercapto-1- propanol	Y. Tanaka <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Five rotamers assigned.
C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> [CO-CH <sub>3</sub> CH(O)CH <sub>2</sub> ]	Carbon monoxide -propylene oxide	H. Mizuno <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	<i>Anti</i> form: normal, <sup>13</sup> CO, C <sup>18</sup> O species, assigned.
C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> [CH <sub>3</sub> CH(CO <sub>3</sub> )CH <sub>2</sub> ]	Propylene carbonate	T. Kinjo <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Normal, <sup>13</sup> C (4 species), <sup>18</sup> O (3 species) assigned.
C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub> [(CH <sub>3</sub> CO) <sub>2</sub> NH]	Diacetamide	Y. Kawashima <sup>a</sup> R. D. Suenram <sup>c</sup> 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 <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> [CH <sub>3</sub> CONHCH <sub>2</sub> CONH <sub>2</sub> ]	<i>N</i> <sub>α</sub> -Acetylglycinamide	Y. Kawashima <sup>a</sup> R. J. Lavrich <sup>c</sup> R. D. Suenram <sup>c</sup> E. Hirota	<i>A</i> state assigned, <i>E</i> state assignment in progress.
C <sub>4</sub> H <sub>9</sub> NO [CH <sub>3</sub> CONHCH <sub>2</sub> CH <sub>3</sub> ]	<i>N</i> -Ethylacetamide	Y. Kawashima <sup>a</sup> T. Usami <sup>a</sup> K. Ohba <sup>a</sup> R. D. Suenram <sup>c</sup> E. Hirota	Manuscript prepared.
C <sub>4</sub> H <sub>10</sub> O [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH]	<i>n</i> -Butanol	T. Uzuyama <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Seven rotamers assigned.
C <sub>4</sub> H <sub>10</sub> O [CH(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> OH]	Isobutanol	T. Uzuyama <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Four rotamers assigned.
C <sub>4</sub> H <sub>10</sub> S [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> SH]	<i>n</i> -Butanethiol	Y. Tanaka <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Seven rotamers, one for SD assigned.
C <sub>4</sub> H <sub>10</sub> S [CH(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> SH]	Isobutanethiol	Y. Tanaka <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Three rotamers, <sup>34</sup> S, <sup>13</sup> C species assigned.
C <sub>5</sub> H <sub>10</sub> O [CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CHOH]	Cyclopentanol	Y. Kawashima <sup>a</sup> E. Hirota B. Carroll <sup>f</sup> G. Blake <sup>f</sup>	Work in progress
C <sub>5</sub> H <sub>12</sub> O [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH]	<i>n</i> -pentanol	Y. Komamine <sup>a</sup> Y. Kawashima <sup>a</sup> 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 <sub>5</sub> H <sub>12</sub> O [H <sub>3</sub> CCH <sub>2</sub> CH(CH <sub>3</sub> )CH <sub>2</sub> OH]	2-Methyl-1-butanol	Y. Kawashima <sup>a</sup> N. Koshimae <sup>a</sup> Y. Tanimoto <sup>a</sup> E. Hirota	Three conformers assigned.
C <sub>5</sub> H <sub>12</sub> S [(CH <sub>3</sub> ) <sub>3</sub> CSCH <sub>3</sub> ]	<i>Tert</i> -butyl methyl sulfide	R. Watanabe <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Normal, <sup>34</sup> S, <sup>13</sup> C species assigned.
C <sub>6</sub> H <sub>10</sub> [CH=CHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ]	Cyclohexene	Y. Kawashima <sup>a</sup> E. Hirota	Isotopomer assigned.
C <sub>6</sub> H <sub>10</sub> O [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CHCHO]	<i>Trans</i> -2-hexenal	R. Yokoyama <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Four conformers assigned
C <sub>6</sub> H <sub>14</sub> O [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH]	<i>n</i> -Hexanol	Y. Hosoya <sup>a</sup> Y. Kawashima <sup>a</sup> E. Hirota	Three conformers assigned
C <sub>8</sub> H <sub>12</sub> [CH=CHCH <sub>2</sub> CH(CH=CH <sub>2</sub> )CH <sub>2</sub> CH <sub>2</sub> ]	4-Vinyl-1-cyclohexene	Y. Nakanishi <sup>a</sup> Y. Kawashima <sup>a</sup> R. J. Lavrich <sup>c</sup> R. D. Suenram <sup>c</sup> 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 <sub>7</sub> H <sub>7</sub> Cl (CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> Cl)	p-chlorotoluene	Ilyushin V. <sup>a,b</sup>	FTMW spectrum of the <sup>35</sup> Cl and <sup>37</sup> Cl isotopologues, analysis in progress
C <sub>3</sub> H <sub>4</sub> O <sub>3</sub> (CH <sub>3</sub> COCOOH)	pyruvic acid	Ilyushin V. <sup>a,c</sup> Alekseev E.	Measurements in the 49-149 GHz range; gs + v <sub>t</sub> =1 state assigned, v <sub>24</sub> in progress.
C <sub>2</sub> H <sub>5</sub> NO (CH <sub>3</sub> CONH <sub>2</sub> )	acetamide	Ilyushin V. <sup>d</sup>	Measurements in the 49-660 GHz range; analysis of v <sub>t</sub> =0,1,2 up to J=60 in progress.
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> COOH)	propionic acid	Ilyushin V. <sup>e</sup>	Microwave spectrum in the 150 – 540 GHz range, v <sub>t</sub> =0 spectrum assigned, ms in preparation.
CH <sub>3</sub> D <sub>2</sub> N (CH <sub>3</sub> ND <sub>2</sub> )	deuterated methylamine	Ilyushin V. <sup>e</sup> Alekseev E.	Measurements in the 50-950 GHz range, spectrum assigned, analysis in progress.
C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	2-furan-methanol	Alekseev E. <sup>e</sup> Dyubko S.	Microwave spectrum in 5 – 210 GHz frequency range, analysis in progress
C <sub>5</sub> H <sub>4</sub> O <sub>3</sub>	2-furan-carboxylic acid	Alekseev E. <sup>e</sup>	Microwave spectra in the 5 - 240 GHz, manuscript in preparation
C <sub>3</sub> H <sub>7</sub> NO (CH <sub>3</sub> CH <sub>2</sub> CONH <sub>2</sub> )	propionamide	Ilyushin V. <sup>e</sup> Alekseev E.	MM+SMM spectra, internal rotation, analysis in progress
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> (HCOOCH <sub>3</sub> )	methylformate	Ilyushin V. <sup>e</sup>	gs and first excited torsional state, 49-950 GHz, v <sub>t</sub> =2 analysis in progress
C <sub>3</sub> H <sub>6</sub> O ((CH <sub>3</sub> ) <sub>2</sub> CO)	acetone	Ilyushin V. <sup>e</sup> Alekseev E.	Measurements in the 49-950 GHz, v <sub>t</sub> =0,1,2 assigned up to J=90, manuscript published J. Mol. Spectrosc. 363 (2019) 111169; v <sub>t</sub> =3,4 analysis in progress.
C <sub>4</sub> H <sub>4</sub> O (CH <sub>3</sub> CCCHO)	2-butylnal	Ilyushin V. <sup>e</sup>	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 <sub>2</sub> H <sub>6</sub> S (CH <sub>3</sub> ) <sub>2</sub> S)	dimethylsulfide	Ilyushin V. <sup>c,e</sup> Aleksseev E.A.	Measurements in the 49 – 660 GHz range, analysis of the $\nu_i=0,1,2$ microwave data up to J=60, published J. Mol. Struct. 1200 (2020) 127114
CH <sub>4</sub> O (CH <sub>3</sub> OH)	methanol	Aleksseev E.	anomalous hyperfine splittings of high J transitions in $\nu_i=2$ , analysis in progress.
C <sub>2</sub> H <sub>4</sub> O (CH <sub>3</sub> CHO)	acetaldehyde	Ilyushin V. <sup>c,e</sup>	Analysis of the $\nu_{10}=1$ and $\nu_i=3,4$ torsional states in the 49 – 960 GHz range is in progress.
C <sub>2</sub> H <sub>4</sub> S (CH <sub>3</sub> CHS)	thio-acetaldehyde	Ilyushin V. <sup>e</sup>	Analysis of the new measurements in the 150 – 660 GHz range, manuscript submitted to J. Mol. Spectrosc.
CH <sub>5</sub> As (CH <sub>3</sub> AsH <sub>2</sub> )	methylarsine	Ilyushin V. <sup>e</sup>	Analysis of the mm and submm spectra up to 650 GHz, manuscript accepted by J. Mol. Struct.
CH <sub>4</sub> S (CH <sub>3</sub> SH)	methyl mercaptan	Ilyushin V. <sup>d</sup>	Measurements in the 49 – 500 GHz range, analysis of the $\nu_i=0,1,2$ microwave data up to J=60, published A&A 629, A73 (2019); $\nu_i=3,4$ and CS stretch + $\angle$ CSH bend MW spectra analysis in progress
CH <sub>4</sub> S (CH <sub>3</sub> <sup>34</sup> SH)	<sup>34</sup> S methyl mercaptan	Ilyushin V. <sup>d</sup>	Measurements in the 49 – 500 GHz range, analysis of the $\nu_i=0,1,2$ states, published A&A 627, A41 (2019)
CH <sub>4</sub> S ( <sup>13</sup> CH <sub>3</sub> SH)	<sup>13</sup> C methyl mercaptan	Ilyushin V. <sup>d</sup>	Measurements in the 49 – 500 GHz range, analysis of the $\nu_i=0,1,2$ , manuscript in press Can. J. Phys.
C <sub>2</sub> H <sub>4</sub> OS (HSCOCH <sub>3</sub> )	O-methyl thioformate	Ilyushin V. <sup>e</sup>	gs and first excited torsional state, 150-650 GHz, analysis in progress.
C <sub>2</sub> H <sub>5</sub> N (CH <sub>3</sub> CHNH)	ethanimine	Ilyushin V. <sup>e</sup>	Measurements in the 75 – 650 GHz range, analysis of E and Z conformers in the $\nu_i=0,1,2$ torsional states in progress
C <sub>2</sub> H <sub>6</sub> O (CH <sub>3</sub> ) <sub>2</sub> O)	dimethylether	Ilyushin V. <sup>f</sup> Aleksseev E.	Measurements in the 34–180 GHz and 265–400 GHz, $\nu_i=0,1,2$ assigned up to J=60, analysis in progress.

<b><u>FORMULA</u></b>	<b><u>NAME OF COMPOUND</u></b>	<b><u>NAME OF INVESTIGATOR</u></b>	<b><u>PRESENT STAGE OF PROGRESS</u></b>
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> (CH <sub>3</sub> COOH)	acetic acid	Ilyushin V.	New measurements in the 145–183 GHz and 265–400 GHz, analysis of the $\nu_i=3,4$ 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>
$H_2N_2O$ ( $oH_2$ -, $pH_2$ -, $pD_2$ - $N_2O$ )	dihydrogen – nitrous oxide	J. N. Landry	Manuscript in preparation. <sup>1</sup>
$H_{2N}N_2O$ , $N=2-12$ ( $oH_2$ ; $pH_2$ ; $^{15}N$ )	(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.
$C_2H_6O_6$ ( $C_2H_2O_4$ -( $H_2O$ ) <sub>2</sub> )	oxalic acid – (water) <sub>2</sub>	E. Schnitzler	Manuscript near completion.
$C_2H_6F_3NO$ ( $C_2H_3F_3O$ - $NH_3$ )	trifluoroethanol-ammonia	J. Thomas I. Peña Y. Yang	Manuscript near completion. <sup>2,3</sup>
$C_2H_{10}O_5$ ( $C_2H_4O_2$ -( $H_2O$ ) <sub>3</sub> )	acetic acid – water <sub>3</sub>	E. Schnitzler N. Seifert	ab initio calculations completed; assignment in progress.
$C_3H_2F_6NeO$ ( $C_3HF_6OH$ -Ne)	hexafluoro-2-propanol – Ne	B. Wu S. Oswald N. Seifert	Manuscript near completion. <sup>2</sup>
$C_3H_2ArF_6O$ ( $C_3HF_6OH$ -Ar)	hexafluoro-2-propanol – Ar	B. Wu S. Oswald N. Seifert	Manuscript near completion. <sup>2</sup>
$C_3H_2F_6N_2O$ ( $C_3HF_6OH$ - $N_2$ )	hexafluoro-2-propanol – $N_2$	S. Oswald N. Seifert B. Wu	Spectra assigned; hyperfine analyses completed. <sup>2,4</sup>

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_3F_5O$	pentafluoro-1-propanol	B. Wu S. Oswald N. Seifert	Detailed fits in progress. <sup>2</sup>
$C_3H_3F_5NeO$ ( $C_3H_3F_5O-Ne$ )	pentafluoro-1-propanol – Ne	B. Wu S. Oswald N. Seifert	Tunneling splittings observed; fits in progress. <sup>2</sup>
$C_3H_4F_6O_2$ ( $C_3H_2F_6-H_2O$ )	hexafluoro-2-propanol – $H_2O$	B. Wu N. Seifert S. Oswald	new conformer assigned. HOD/DOH/ $D_2O$ analyses completed. <sup>2</sup>
$C_3H_5F_5O_2$ ( $C_3H_3F_5O$ )- $H_2O$	pentafluoro-1-propanol – water	B. Wu N. Seifert S. Oswald	Two conformers assigned; isotopic analyses completed; manuscript in preparation. <sup>2</sup>
$C_3H_8O_2$ ( $C_3H_6O-H_2O$ )	acetone – water	J. Gao J. Thomas	Manuscript near completion. <sup>2</sup>
$C_3H_8O_3$ ( $C_3H_6O_2-H_2O$ )	hydroxyacetone – water	E. Schnitzler N. Seifert J. Thomas	ab initio calculations completed; assignment in progress.
$C_4H_4N_2O$	4-hydroxypyrimidine	J. Gao	Two tautomers identified.
$C_4H_4O_2$	2-furanol	X. Dong N. Seifert	ab initio calculations completed; assignment in progress.
$C_4H_6N_2O_2$ ( $C_4H_4N_2O-H_2O$ )	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. <sup>2</sup>
$C_4H_9F_3O_2$ ( $C_4H_7F_3O-H_2O$ )	4,4,4-trifluorobutanol – water	T. Lu F. Xie	Assignment in progress. <sup>2</sup>
$C_4H_9NO_2$ ( $C_4H_5N-(H_2O)_2$ )	pyrrole – (water) <sub>2</sub>	B. Wu J. Thomas	ab initio calculations; assignment in progress. <sup>2</sup>
$C_5H_5He_N N$ ( $N=1-19$ ) ( $C_5H_5N-He_N$ )	pyridine – $He_N$ ( $N=1-19$ )	A. Hazrah N. Seifert	Spectra assigned; manuscript in preparation. <sup>5</sup>

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>5</sub> H <sub>5</sub> N <sub>3</sub> (C <sub>5</sub> H <sub>5</sub> N-N <sub>2</sub> )	pyridine – nitrogen	C. Tanjaroon	Manuscript in preparation.
C <sub>5</sub> H <sub>7</sub> N (C <sub>5</sub> H <sub>5</sub> N-H <sub>2</sub> )	pyridine – hydrogen	C. Tanjaroon	Manuscript in preparation.
C <sub>5</sub> H <sub>10</sub> O <sub>3</sub> (C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> -H <sub>2</sub> O)	acetylacetone – water	J. Gao	ab initio calculations completed; partial assignment.
C <sub>5</sub> H <sub>10</sub> O <sub>4</sub> (C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> -H <sub>2</sub> O)	tetrahydro-2-furoic acid - water	F. Xie S. Mahendiran	Spectra assigned; manuscript in preparation. <sup>2</sup>
C <sub>5</sub> H <sub>11</sub> N	2-methylpyrrolidine	T. Lu A. Harah	Two conformers assigned; ab initio calculations completed.
C <sub>5</sub> H <sub>13</sub> NO (C <sub>5</sub> H <sub>11</sub> N-H <sub>2</sub> O)	2-methylpyrrolidine – water	T. Lu A. Harah	Spectral assignment underway; ab initio calculations completed.
C <sub>6</sub> H <sub>6</sub> F <sub>6</sub> O <sub>2</sub> (C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O) <sub>2</sub>	Trifluoromethyl oxirane dimer	H. Leung M. Marshall N. Seifert	Spectra assigned; manuscript in preparation. <sup>2,6</sup>
C <sub>6</sub> H <sub>6</sub> F <sub>10</sub> O <sub>2</sub> (C <sub>3</sub> H <sub>3</sub> F <sub>5</sub> O) <sub>2</sub>	pentafluoro-1-propanol dimer	S. Oswald B. Wu N. Seifert	Five dimers assigned; manuscript in preparation. <sup>2</sup>
C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> (C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> -H <sub>2</sub> O)	1,3-cyclohexanedione – H <sub>2</sub> O	J. Gao	ab initio calculations completed; assignment in progress.
C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> ((C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ) <sub>2</sub> )	(hydroxyacetone) <sub>2</sub>	E. Schnitzler N. Seifert J. Thomas	ab initio calculations completed; assignment in progress.
C <sub>6</sub> H <sub>16</sub> O <sub>6</sub> ((C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> ) <sub>2</sub> )	glycerol dimer (propane-1,2,3-triol) <sub>2</sub>	F. Xie N. Seifert	Several dimers assigned. <sup>2</sup>
C <sub>7</sub> H <sub>5</sub> He <sub>N</sub> (N=1- 8) (C <sub>7</sub> H <sub>5</sub> N-He <sub>N</sub> )	benzonitrile – He <sub>N</sub> (N=1-8)	A. Hazrah N. Seifert	Spectra assigned; manuscript in preparation. <sup>5</sup>
C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	3-methylcatechol	A. Hazrah	ab initio calculations completed; assignment in progress.
C <sub>7</sub> H <sub>10</sub> O <sub>3</sub> (C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> -H <sub>2</sub> O)	3-methylcatechol – water	A. Hazrah	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>
$C_7H_{12}O_2$	cyclohexanecarboxylic acid	T. Lu A. Hazrah F. Xie	One conformer assigned; others in progress. <sup>2,7</sup>
$C_7H_{14}O_3$ ( $C_7H_{12}O_2$ )- $H_2O$	cyclohexanecarboxylic acid – water	T. Lu A. Hazrah F. Xie	One conformer assigned; others in progress. <sup>2,7</sup>
$C_8H_8O_4$	vanillic acid	M. Al-Jabiri	Spectra assigned; ab initio calculations completed
$C_8H_{10}O_3$ ( $C_8H_8O_2$ - $H_2O$ )	<i>m</i> -toluic acid – water	E. Schnitzler N. Seifert M. Al-Jabiri	ab initio calculations completed; assignment in progress.
$C_8H_{10}O_5$ ( $C_8H_8O_4$ )- $H_2O$	vanillic acid – water	M. Al-Jabiri	Spectra assigned; ab initio calculations completed.
$C_8H_{11}NO_3$ ( $C_8H_8O_3$ - $NH_3$ )	methyl salicylate – ammonia	J. Thomas J. Kwak	ab initio calculations completed; assignment in progress. <sup>2</sup>
$C_8H_{12}F_{12}O_4$ ( $C_2H_3F_3O$ ) <sub>4</sub>	trifluoroethanol tetramer	J. Thomas N. Seifert	Assignment in progress. <sup>2</sup>
$C_8H_{14}F_6O_2$ ( $C_4H_7F_3O$ ) <sub>2</sub>	4,4,4-trifluorobutanol dimer	T. Lu F. Xie	Conformational search complete one conformer assigned. <sup>2</sup>
$C_9H_{10}O_4$	3,4-dimethoxybenzoic acid (veratric acid)	M. Al-Jabiri	Spectra assigned; ab initio calculations completed.
$C_9H_{12}O_5$	veratric acid – water	M. Al-Jabiri	Spectra assigned; ab initio calculations completed.
$C_9H_{18}O_3$ ( $(C_3H_6O)_3$ )	propylene oxide trimer	F. Xie A. Hazrah	Several conformers assigned; manuscript near completion. <sup>2,8</sup>
$C_{10}H_8O$	2-naphthalenethiol	A. Hazrah	Two conformers assigned.
$C_{10}H_8O$	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 completed; 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 completed; assignment completed.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{10}H_{16}O$	carveol	A. Hazrah	Six conformers assigned.
$C_{10}H_{16}O_6$ $((C_5H_8O_3)_2)$	(tetrahydro-2-furoic acid) <sub>2</sub>	F. Xie N. Seifert	Dimer assigned; manuscript in preparation. <sup>2</sup>
$C_{10}H_{18}O$ $(C_{10}H_{16}-H_2O)$	$\alpha$ -pinene – water	A. Hazrah	ab initio calculations completed; assignment in progress.
$C_{10}H_{18}O_2$ $(C_{10}H_{16}O-H_2O)$	perillyl alcohol – water	F. Xie N. Seifert	Assignment in progress. <sup>2</sup>
$C_{10}H_{18}O_4$ $(C_{10}H_{16}O_3-H_2O)$	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.
$C_{12}H_{21}F_9O_3$ $(C_4H_7F_3O)_3$	4,4,4-trifluorobutanol trimer	T. Lu F. Xie	Conformational search complete one conformer assigned. <sup>2</sup>

<sup>1</sup> In collaboration with Professor Yasuki Endo, National Chiao Tung University, Taiwan.

<sup>2</sup> In collaboration with Professor Yunjie Xu, University of Alberta, Canada.

<sup>3</sup> In collaboration with Dr. Isabelle Peña, Universidad de Valladolid, Spain.

<sup>4</sup> In collaboration with Professor Martin Suhm, University of Göttingen, Germany.

<sup>5</sup> In collaboration with Professor Paul Raston, James Madison University, USA.

<sup>6</sup> In collaboration with Professor Helen Leung and Professor Mark Marshall, Amherst College, USA.

<sup>7</sup> In collaboration with Professor Q. Gou and Professor G. Feng, Chongqing University, China.

<sup>8</sup> In collaboration with Dr. M. Fusè and Professor Vincent Barone, Scuola Normale Superiore, Italy.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>2</sub> F <sub>6</sub> O <sub>2</sub>	Bis(trifluoromethyl) peroxide	Kang; Novick	Presentation in ISMS
<sup>13</sup> C <sub>2</sub> F <sub>6</sub> O <sub>2</sub>	<sup>13</sup> C isotopologue	Kang; Novick	Searching for <sup>18</sup> O-iso
C <sub>2</sub> F <sub>2</sub> N	1,1-difluorocyanomethyl radical	Kang; Novick	Spectrum assigned
C <sub>3</sub> F <sub>6</sub> O	Hexafluoropropylene	Kang; Shipman; Pate	Presentation in ISMS Spectrum assigned
C <sub>4</sub> DNO <sub>2</sub>	Deuterated T-shaped carbon dioxide cyanoacetylene complex	Kang; Novick; Kukolich	Presentation in ISMS Transitions observed
C <sub>3</sub> HN <sub>3</sub>	Linear nitrogen-cyanoacetylene complex	Kang; Novick	working on hf structures Spectrum assigned
C <sub>6</sub> HDN <sub>2</sub>	HCCCN---DCCCN complex	Kang; Novick; Kukolich	working on hf structures Spectrum assigned
C <sub>6</sub> HDN <sub>2</sub>	DCCCN---HCCCN complex	Kang; Novick; Kukolich	working on hf structures Spectrum assigned
C <sub>6</sub> D <sub>2</sub> N <sub>2</sub>	DCCCN dimer complex	Kang; Novick; Kukolich	working on hf structures Spectrum assigned
C <sub>3</sub> F <sub>6</sub> O	Perfluoromethylvinylether	Kang; Brown; Pate	working on hf structures Spectrum assigned
C <sub>7</sub> H <sub>3</sub> F <sub>5</sub> O	2,3,4,5,6-perfluoroansiol	Kang; Pate	Spectrum assigned
C <sub>3</sub> H <sub>10</sub> Si	Trimethylsilane	Kang; Novick	Spectrum assigned
C <sub>5</sub> H <sub>10</sub> Si	Trimethylsilylacetylene	Kang; Novick	Manuscript in preparation Spectrum assigned
C <sub>7</sub> H <sub>10</sub> Si	Trimethylsilyldiacetylene	Kang; Novick	Presentation in ISMS Manuscript in preparation
C <sub>6</sub> H <sub>9</sub> NSi	Trimethylsilylacetylene cyanide	Kang; Novick	Spectrum assigned Presentation in ISMS
C <sub>3</sub> H <sub>3</sub> NSi	Silylacetylene cyanide	Kang; Novick	Manuscript in preparation 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 <sub>4</sub> Li [LiBH <sub>4</sub> ]	Lithium tetrahydroborate	Y. Kawashima E. Hirota <sup>a</sup>	Excited vibrational states, work in progress.
BH <sub>4</sub> K [KBH <sub>4</sub> ]	Potassium tetrahydroborate	Y. Kawashima E. Hirota <sup>a</sup>	Excited vibrational states, work almost completed.
CH <sub>6</sub> O [CD <sub>4</sub> -- H <sub>2</sub> O, HDO, D <sub>2</sub> O]	Methane-water	Y. Kawashima L.H.Coudert <sup>c</sup>	Manuscript prepared
C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O [N <sub>2</sub> -(CH <sub>3</sub> ) <sub>2</sub> O]	Dinitrogen-dimethyl ether	Y. Kawashima E. Hirota <sup>a</sup>	Spectra assigned for N <sub>2</sub> , N <sup>15</sup> N, <sup>15</sup> N <sub>2</sub> species.
C <sub>3</sub> H <sub>5</sub> NO [CH <sub>2</sub> =CHCONH <sub>2</sub> ]	Acrylamide	T. Usami Y. Kawashima	Isotopomers assigned
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> [NH <sub>2</sub> COCH <sub>2</sub> CONH <sub>2</sub> ]	Malonamide	T. Usami E. Hirota <sup>a</sup> R. D. Suenram <sup>b</sup>	Manuscript prepared.
C <sub>3</sub> H <sub>6</sub> O [CH <sub>3</sub> CH(O)CH <sub>2</sub> ]	Propylene oxide	E. Hirota <sup>a</sup> Y. Kawashima	Work completed.
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S [CO <sub>2</sub> -(CH <sub>3</sub> ) <sub>2</sub> S]	Carbon dioxide-dimethyl-sulfide	Y. Kawashima S. Iwano E. Hirota <sup>a</sup>	Work in progress, two states assigned.
C <sub>3</sub> H <sub>7</sub> NO [HCONHCH <sub>2</sub> CH <sub>3</sub> ]	<i>N</i> -Ethylformamide	K. Ohba T. Usami Y. Kawashima E. Hirota <sup>a</sup>	Second conformer assigned.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>3</sub> H <sub>8</sub> OS [OHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> SH]	3-Mercapto-1- propanol	Y. Tanaka Y. Kawashima E. Hirota <sup>a</sup>	Five rotamers assigned.
C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> [CO-CH <sub>3</sub> CH(O)CH <sub>2</sub> ]	Carbon monoxide -propylene oxide	Y. Kawashima H. Mizuno E. Hirota <sup>a</sup>	<i>Anti</i> form: normal, <sup>13</sup> C, C <sup>18</sup> O species, assigned.
C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> [CH <sub>3</sub> CH(CO <sub>3</sub> )CH <sub>2</sub> ]	Propylene carbonate	T. Kinjo Y. Kawashima E. Hirota <sup>a</sup>	Normal, <sup>13</sup> C (4 species), <sup>18</sup> O (3 species) assigned.
C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub> [(CH <sub>3</sub> CO) <sub>2</sub> NH]	Diacetamide	Y. Kawashima R. D. Suenram <sup>b</sup> E. Hirota <sup>a</sup>	<i>A</i> state and <i>E</i> state assigned.
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> [CH <sub>3</sub> CONHCH <sub>2</sub> CONH <sub>2</sub> ]	N <sub>α</sub> -Acetylglycinamide	Y. Kawashima R. J. Lavrich <sup>d</sup> R. D. Suenram <sup>b</sup> E. Hirota <sup>a</sup>	<i>A</i> state assigned, <i>E</i> state assignment in progress.
C <sub>4</sub> H <sub>9</sub> NO [CH <sub>3</sub> CONHCH <sub>2</sub> CH <sub>3</sub> ]	N-Ethylacetamide	T. Usami K. Ohba Y. Kawashima R. D. Suenram <sup>b</sup> E. Hirota <sup>a</sup>	Manuscript prepared.
C <sub>4</sub> H <sub>10</sub> O [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH]	<i>n</i> -Butanol	T. Uzuyama Y. Kawashima E. Hirota <sup>a</sup>	Seven rotamers assigned.
C <sub>4</sub> H <sub>10</sub> O [CH(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> OH]	Isobutanol	T. Uzuyama Y. Kawashima E. Hirota <sup>a</sup>	Four rotamers assigned.
C <sub>4</sub> H <sub>10</sub> S [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> SH]	<i>n</i> -Butanethiol	Y. Tanaka Y. Kawashima E. Hirota <sup>a</sup>	Seven rotamers, one for SD assigned.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>10</sub> S [CH(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> SH]	Isobutanethiol	Y. Tanaka Y. Kawashima E. Hirota <sup>a</sup>	Three rotamers, <sup>34</sup> S, <sup>13</sup> C species assigned.
C <sub>5</sub> H <sub>10</sub> O [CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CHOH]	Cyclopentanol	Y. Kawashima E. Hirota <sup>a</sup> B. Carroll <sup>f</sup> G. Blake <sup>f</sup>	Work in progress
C <sub>5</sub> H <sub>12</sub> O [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH]	<i>n</i> -pentanol	Y. Kawashima Y. Komamine E. Hirota <sup>a</sup>	Six isomers assigned.
C <sub>5</sub> H <sub>12</sub> O [H <sub>3</sub> CCH <sub>2</sub> CH(CH <sub>3</sub> )CH <sub>2</sub> OH]	2-Methyl-1-butanol	Y. Kawashima N. Koshimae Y. Tanimoto E. Hirota <sup>a</sup>	Three conformers assigned.
C <sub>5</sub> H <sub>12</sub> S [(CH <sub>3</sub> ) <sub>3</sub> CSCH <sub>3</sub> ]	<i>Tert</i> -butyl methyl sulfide	Y. Kawashima R. Watanabe E. Hirota <sup>a</sup>	Normal, <sup>34</sup> S, <sup>13</sup> C species assigned.
C <sub>6</sub> H <sub>6</sub> O [(HCCCH <sub>2</sub> ) <sub>2</sub> O]	Dipropargyl ether	T. Usami Y. Kawashima	Work almost completed
C <sub>6</sub> H <sub>6</sub> S [C <sub>6</sub> H <sub>5</sub> SH]	Thiophenol	R. Jono <sup>e</sup> A. Hino <sup>e</sup> M. Onda <sup>e</sup> Y. Kawashima	Normal, D, <sup>34</sup> S, <sup>13</sup> C species assigned
C <sub>6</sub> H <sub>10</sub> [CH=CHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ]	Cyclohexene	Y. Kawashima E. Hirota <sup>a</sup>	Isotopomer assigned.
C <sub>6</sub> H <sub>10</sub> O [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CHCHO]	<i>Trans</i> -2-hexenal	R. Yokoyama Y. Kawashima E. Hirota <sup>a</sup>	Four conformers assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> [O(CO)CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>2</sub> CH <sub>3</sub> )]	γ-Hexanolactone	T. Takimoto <sup>c</sup> N. Kuze <sup>e</sup> Y. Kawashima	Three conformers assigned
C <sub>6</sub> H <sub>14</sub> O [CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH]	<i>n</i> -Hexanol	Y. Hosoya Y. Kawashima E. Hirota <sup>a</sup>	Three conformers assigned
C <sub>8</sub> H <sub>12</sub> [CH=CHCH <sub>2</sub> CH(CH=CH <sub>2</sub> )CH <sub>2</sub> CH <sub>2</sub> ]	4-Vinyl-1-cyclohexene	Y. Nakanishi Y. Kawashima R. J. Lavrich <sup>d</sup> R. D. Suenram <sup>b</sup> E. Hirota <sup>a</sup>	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 <sub>3</sub> O (H <sub>2</sub> O...HBr)	Water...hydrogen bromide	BP, OD, LP, ZK, <i>Bri</i>	FTMW: isotopic work+dipole moment - completed, ms. in prep.
Cl <sub>2</sub> H <sub>6</sub> O <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> (HCl) <sub>2</sub>	Water...hydrogen chloride (2/2)	<i>Vir</i> , ZK	Assigned in chirped pulse FTMW, ms. in prep.
ClH <sub>7</sub> O <sub>3</sub> (H <sub>2</sub> O) <sub>3</sub> HCl	Water...hydrogen chloride (3/1)	<i>Vir</i> , ZK	Assigned in chirped pulse FTMW, ms in prep.
H <sub>12</sub> O <sub>6</sub> (H <sub>2</sub> O) <sub>6</sub>	Water hexamer	<i>Vir</i> , ZK	All 64 combinations of <sup>16</sup> O/ <sup>18</sup> O for each of three hexamer conformers observed and analysed.
FH <sub>3</sub> O (H <sub>2</sub> O...HF)	Water...hydrogen fluoride	ZK, <i>NN</i>	MMW spectrum, new analysis
ArClH <sub>3</sub> O (H <sub>2</sub> O...HCl)...Ar	(Water...hydrogen chloride)...argon	EBJ, ZK, LP, <i>Vir</i>	FTMW (Balle-Flygare and chirped pulse): parent+D+ <sup>37</sup> Cl+ <sup>18</sup> O, dipole moment, ms. in prep.
CH <sub>4</sub> N <sub>2</sub> O (NH <sub>2</sub> ) <sub>2</sub> C=O	Urea	<i>Koln</i> , <i>Wri</i> , ZK	Astrophysical detection, <i>A&amp;A</i> <b>628</b> , A10(2019); Lab spectroscopy of g.s.+ excited vibrational states, in prep.
C <sub>4</sub> H <sub>7</sub> Cl (C <sub>4</sub> H <sub>6</sub> ...HCl)	1,3-butadiene...hydrogen chloride	ZK, <i>Bri</i>	FTMW: partial assignment
C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O	2-aminopyridine... H <sub>2</sub> O cyclic dimer	AK, EBJ, ZK, LP, <i>Rennes</i>	FTMW: nearing completion, more isotopic species measured
C <sub>2</sub> Cl <sub>3</sub> N Cl <sub>3</sub> CCN	Trichloroacetonitrile	ZK, LP, EBJ	FTMW: hyperfine from 4 nuclei resolved and fitted
C <sub>2</sub> Cl <sub>4</sub> F <sub>2</sub> Cl <sub>3</sub> CCClF <sub>2</sub>	CFC-112a	<i>Bilbao</i> , EBJ, ZK	Chirped pulse+cavity FTMW, 4xCl hyperfine and isotopic species analysed
C <sub>2</sub> H <sub>3</sub> NO CH <sub>3</sub> NCO	Methyl isocyanate	<i>Val</i> , <i>Rennes</i> , ZK	Further parent transitions + <sup>13</sup> C, <i>ApJSS</i> <b>245</b> ,31(2019); Work continuing.



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>2</sub> H <sub>3</sub> NS CH <sub>3</sub> NCS	Methyl isothiocyanate	Ohio, ZK	FASSST spectrum partially analysed
C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O H <sub>2</sub> NCH <sub>2</sub> CONH <sub>2</sub>	Glycine amide	ZK, LP, Rennes, Val	MMW, inversion, vibr.satellites: ms in prep.
C <sub>3</sub> H <sub>3</sub> N H <sub>2</sub> C=CHCN	Acrylonitrile	Par, ZK, LP	FTIR+MMW+SMM, excited vibr. states >600 cm <sup>-1</sup>
C <sub>2</sub> H <sub>7</sub> N C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	Ethylamine	Ohio, AK, ZK, Koln	Spectrum up to 1 THz, torsion + inversion analysis in prog.
C <sub>3</sub> H <sub>8</sub> O <sub>4</sub> , C <sub>3</sub> H <sub>10</sub> O <sub>5</sub> , C <sub>3</sub> H <sub>12</sub> O <sub>6</sub>	LacticAcid+H <sub>2</sub> O LacticAcid+(H <sub>2</sub> O) <sub>2</sub> LacticAcid+ (H <sub>2</sub> O) <sub>3</sub>	Vir, ZK,EBJ	Chirped pulse FTMW: clusters of lactic acid with H <sub>2</sub> O and two lactide conformers, ms. in prep.
C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>	Lactide		
C <sub>3</sub> H <sub>8</sub> O CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> OH	<i>n</i> -propanol	ZK, Ohio, JPL	<i>T</i> series of conformers: in progress
CH <sub>2</sub> Cl <sub>2</sub> C <sub>3</sub> H <sub>2</sub> ClN C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	Methylene chloride 2-chloroacrylonitrile Pyrimidine	OD, ZK, Bold	FTMW: dipole moment from Stark effect under resolved hfs from two quadrupolar nuclei
C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>	2-Aminopyridine	ZK, LP	MMW+FTMW: c.d., hyperfine, g.s. + inversion satellite
C <sub>5</sub> H <sub>8</sub>	Isoprene	ZK, LP, JPL, Par, Har	MMW+FTMW+FTIR: parent+satellites, ms in prep.
C <sub>5</sub> H <sub>12</sub> O (CH <sub>3</sub> ) <sub>3</sub> CCH <sub>2</sub> OH	Neopentyl alcohol	LP, ZK, Goet	MMW+FTMW: two conformers assigned
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	1,2-dichlorobenzene	ZK, LP, EBJ	Chirped pulse FTMW+MMW, g.s.+isotopes+vibrational satellites+structure, ms in prep.
C <sub>6</sub> H <sub>5</sub> F C <sub>8</sub> H <sub>6</sub>	Fluorobenzene Phenylacetylene	ZK, EBJ	Sextic cd from WG-FTMW in CMW region <i>JMS</i> <b>359</b> ,16(2019),.
C <sub>7</sub> H <sub>5</sub> N	Benzonitrile	Wisc, ZK	Higher vibrational states, in prog.
C <sub>7</sub> H <sub>7</sub> Cl	<i>p</i> -chlorotoluene	Kha, Han, ZK,	Low-barrier sixfold internal rotation with hyperfine, in prog.
C <sub>8</sub> H <sub>7</sub> N	<i>p</i> -Cyanotoluene	EBJ, ZK, LP	MMW+FTMW: c.d. + internal rot., in progress
C <sub>10</sub> H <sub>16</sub> O,	Thujone	Hamb, ZK	Chirped pulse FTMW, heavy atom molecular backbones from <sup>13</sup> C and <sup>18</sup> O in natural abundance.
C <sub>10</sub> H <sub>18</sub> O <sub>2</sub> , C <sub>10</sub> H <sub>20</sub> O <sub>3</sub>	Thujone+H <sub>2</sub> O Thujone+(H <sub>2</sub> O) <sub>2</sub>		Several cluster conformers assigned.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>10</sub> H <sub>15</sub> F	1-fluoro-adamantane	BP, ZK, LP, <i>Bri</i>	MMW + FTMW, electric dipole moment, completed
C <sub>10</sub> H <sub>15</sub> Cl	1-chloro-adamantane		
C <sub>10</sub> H <sub>15</sub> Br	1-bromo-adamantane		
C <sub>10</sub> H <sub>15</sub> I	1-iodo-adamantane		
CINO <sub>3</sub>	ClONO <sub>2</sub>	Chlorine nitrate	<i>Ohio</i> , ZK, EBJ
			FASSST spectrum: further vibrational satellites in prog.
HN <sub>3</sub>	Hydrazoic acid	<i>Pra</i> , <i>Wisc</i> , ZK	Broadband MMW+SMM: analysis of higher states in prog.
ANALYSIS/DATABASE	Programs for ROTational SPEctroscopy- PROSPE <a href="http://info.ifpan.edu.pl/~kisiel/prospe.htm">http://info.ifpan.edu.pl/~kisiel/prospe.htm</a>		
ANALYSIS/DATABASE	Worked examples of various fitting programs: <a href="http://info.ifpan.edu.pl/~kisiel/data.htm">http://info.ifpan.edu.pl/~kisiel/data.htm</a>		

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A database "Programs for ROTational SPEctroscopy (PROSPE)" is available at:

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

Many data files serving as worked examples of the use of various fitting programs are available at:

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

A subpage on this Newsletter is at:

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH <sub>4</sub> O (CH <sub>3</sub> OH, <sup>13</sup> CH <sub>3</sub> OH CH <sub>3</sub> <sup>18</sup> OH, CH <sub>3</sub> OD)	Methanol	F. Matsushima K. Kobayashi	ground and CO stretching vibrational state, far infrared spectrum and Zeeman effect
CH <sub>4</sub> S  (CH <sub>3</sub> SH, CD <sub>3</sub> SH)	Methanethiol	K. Kobayashi	mm-wave spectrum  1st and 2nd excited torsional states assigned Manuscript on the ground and 1 <sup>st</sup> excited states was submitted to J. Mol. Structure.
CH <sub>5</sub> N  (CH <sub>3</sub> NH <sub>2</sub> )	Methylamine	K. Kobayashi	mm-wave spectrum  prep. spectrum atlas
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> (HCOOCH <sub>3</sub> , DCOOCH <sub>3</sub> , H <sup>13</sup> COOCH <sub>3</sub> HCOO <sup>13</sup> CH <sub>3</sub> )	Methyl formate	K. Kobayashi <sup>1,2</sup>	HCOOCH <sub>3</sub> , two new vibrational states (one state was assigned to ν <sub>12</sub> ) assigned far-infrared spectrum Manuscript on ν <sub>12</sub> was accepted to Can. J. Phys.
C <sub>2</sub> H <sub>6</sub> O (C <sub>2</sub> H <sub>5</sub> OH)	Ethanol	K. Kobayashi	spectrum assigned
C <sub>2</sub> O ( <sup>13</sup> CCO, C <sup>13</sup> CO, <sup>13</sup> C <sup>13</sup> CO, CC <sup>18</sup> O)	Ketenylidene	K. Kobayashi <sup>3</sup>	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 <sub>3</sub> H <sub>3</sub> NO	Isoxazole Oxazole	K. Kobayashi	ground state assigned in preparation of the manuscript
C <sub>3</sub> H <sub>3</sub> NS	Isothiazole	K. Kobayashi	ground state assigned
C <sub>3</sub> H <sub>5</sub> N (CH <sub>3</sub> CH <sub>2</sub> CN)	Ethyl cyanide	Y. Fukuyama <sup>4</sup> K. Kobayashi H. Odashima <sup>5</sup>	prep. spectrum atlas
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> (CH <sub>3</sub> COOCH <sub>3</sub> )	Methyl Acetate	K. Kobayashi <sup>6</sup> I. Kleiner <sup>7</sup>	mm-wave spectrum
C <sub>3</sub> H <sub>8</sub> O (CH <sub>3</sub> OC <sub>2</sub> H <sub>5</sub> )	Ethyl methyl ether	K. Kobayashi <sup>1,2</sup>	mm-wave spectrum ground and excited states assigned (skeletal torsion vt=2,3)
C <sub>4</sub> H <sub>4</sub> S	Thiophene	K. Kobayashi	40-170 GHz spectrum assigned
CaH	Calcium Monohydride	F. Matsushima, K. Kobayashi	Terahertz spectra assigned
H <sub>2</sub> N (NHD)	Amidogen	K. Kobayashi <sup>8</sup>	Terahertz spectra in preparation of the manuscript

1. In collaboration with M. Fujitake and N. Ohashi (Kanazawa University, Japan).
2. In collaboration with D. W. Tokaryk (University of New Brunswick, Canada) and Brant E. Billingham (Canadian Light Source, Inc., University of Saskatchewan, Canada).
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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<b><u>FORMULA</u></b>	<b><u>NAME OF COMPOUND</u></b>	<b><u>NAMES OF INVESTIGATORS</u></b>	<b><u>PRESENT STAGE OF PROGRESS</u></b>
<b>C<sub>6</sub>H<sub>3</sub>MnO<sub>6</sub></b>	Methylmanganese Pentacarbonyl	C. Tanjaroan, Z. Zhou, D. Mills, K. Keck, and S. G. Kukolich	<i>Inorganic Chemistry</i> April 22, (2020)
<b>C<sub>2</sub>H<sub>6</sub>N<sub>2</sub>O<sub>6</sub></b>	Formamidinium Formate	Z. Zhou, R. Aitken, C. Cardinaud, A. Slawin, H. Wang, A. Daly, M. Palmer, S. Kukolich	<i>J. Chem. Phys.</i> <b>150</b> , 094305 (2019)
<b>C<sub>2</sub>H<sub>6</sub><sup>15</sup>N<sub>2</sub>O<sub>6</sub></b>	Formamidinium Formate ( <sup>15</sup> N)	Z. Zhou, R. Aitken, S. Kukolich	New spectra measured and assigned.
<b>C<sub>6</sub>H<sub>6</sub>BCl</b>	1-Chloroborepin	A. M. Pejlovas, Z. Zhou, A. Ashe III, S. G. Kukolich	<i>J. Phys. Chem. A.</i> <b>122</b> (6) 1542-1549 (2018)
<b>C<sub>9</sub>H<sub>6</sub>O<sub>2</sub></b>	Phenylpropionic Acid	Aaron M. Pejlovas, Zunwu Zhou, Wei Lin, Stephen G. Kukolich	<i>J. Mol. Spectrosc.</i> <b>338</b> , 1-3 (2018)
<b>C<sub>10</sub>H<sub>8</sub>O<sub>4</sub></b>	Phenylpropionic Acid – Formic Acid Dimer	Aaron M. Pejlovas, Zunwu Zhou, Wei Lin, Stephen G. Kukolich	Scanning in progress
<b>C<sub>10</sub>H<sub>8</sub>O<sub>4</sub></b>	Benzoic Acid - propionic Acid –Dimer	Lily Taylor, Adam Daly	Scanning in progress Measured lines
<b>C<sub>9</sub>H<sub>12</sub>FeO</b>	Dibutadiene Iron carbonyl	David Mills, Stephen G. Kukolich	Scanning in progress Measured lines

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<u>FORMULA</u>		<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CF <sub>2</sub> NOPS	F <sub>2</sub> P(S)-NCO	Difluorothiophosphoryl isocyanate	S. Watanabe N. Kuze	Spectrum assigned.
CF <sub>2</sub> NPS <sub>2</sub>	F <sub>2</sub> P(S)-NCS	Difluorothiophosphoryl isothiocyanate	S. Watanabe N. Kuze	Spectrum assigned.
C <sub>2</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	(CH <sub>3</sub> OC(=O)N <sub>3</sub> )	Methyl azidoformate	S. Watanabe N. Kuze	Spectrum assigned.
C <sub>3</sub> H <sub>3</sub> NO <sub>3</sub>	(CH <sub>3</sub> OC(=O)NCO)	Methoxycarbonyl isocyanate	S. Watanabe N. Kuze	Manuscript in prep.
C <sub>3</sub> H <sub>5</sub> NO	(CH <sub>3</sub> CH <sub>2</sub> -OCN)	Ethyl cyanate	T. Sakaizumi N. Kuze	Manuscript in prep.
C <sub>3</sub> H <sub>5</sub> NO	(CH <sub>3</sub> CH=CH-NO)	1- Nitrosopropene	T. Sakaizumi N. Kuze	<i>V</i> <sub>3</sub> (ν=1) determined. Manuscript in prep.
C <sub>4</sub> H <sub>7</sub> NO	$\overbrace{(\text{HNCH}_2(\text{CH}_2)_2\text{C}=\text{O})}$	2-Pyrrolidone	N. Kuze	Manuscript in prep.
C <sub>4</sub> H <sub>7</sub> NO	$\overbrace{(\text{CH}_2(\text{CH}_2)_2\text{C}=\text{NOH})}$	Cyclobutanone oxime	E. Sato N. Kuze	Manuscript in prep.
C <sub>4</sub> H <sub>9</sub> NO	(CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> CH=NOH)	(Z)- <i>n</i> -Butyraldehyde oxime	O. Ohashi N. Kuze	Observation of hyper-fine structure
C <sub>6</sub> H <sub>11</sub> NO	$\overbrace{(\text{HNCH}_2(\text{CH}_2)_4\text{C}=\text{O})}$	ε-Caprolactam	N. Kuze	Manuscript in prep.
C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	(CH <sub>3</sub> ) <sub>3</sub> C(=O)COCH <sub>3</sub> )	Methyl Trimethylacetate	N. Kuze	Spectra for <sup>13</sup> C species were assigned.
C <sub>6</sub> H <sub>11</sub> NO	$\overbrace{(\text{OC}(\text{=O})(\text{CH}_2)_2\text{CH}-\text{C}_2\text{H}_5)}$	γ-Hexanolactone	T. Takimoto	Spectrum assigned.
C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OCOCH <sub>3</sub>	Benzyl acetate	N. Kuze	Spectrum assigned.



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>2</sub> H <sub>4</sub> AgF*	C <sub>2</sub> H <sub>4</sub> ···Ag–F	S. L. Stephens	Spectrum assigned.
C <sub>2</sub> H <sub>4</sub> AgI*	C <sub>2</sub> H <sub>4</sub> ···Ag–I	S. L. Stephens	Spectrum assigned.
C <sub>2</sub> H <sub>4</sub> AuI*	C <sub>2</sub> H <sub>4</sub> ···Au–I	S. L. Stephens, M. Sprawling, D. P. Zaleski	Spectra of isotopologues assigned.
C <sub>2</sub> H <sub>4</sub> CuF*	C <sub>2</sub> H <sub>4</sub> ···Cu–F	S. L. Stephens	Spectrum assigned.
C <sub>2</sub> H <sub>4</sub> CuI*	C <sub>2</sub> H <sub>4</sub> ···Cu–I	S. L. Stephens	Spectrum assigned.
C <sub>2</sub> H <sub>3</sub> BrS	(CH <sub>2</sub> ) <sub>2</sub> S···H–Br	S. Batten	<sup>13</sup> C and <sup>34</sup> S species assigned.
C <sub>3</sub> H <sub>2</sub> F <sub>3</sub> I*	C <sub>2</sub> H <sub>2</sub> ···ICF <sub>3</sub>	S. L. Stephens	Manuscript in preparation
C <sub>3</sub> H <sub>4</sub> ArN <sub>2</sub> *	Imidazole···Ar	E. Gougoula	Manuscript in preparation
C <sub>3</sub> H <sub>9</sub> AgIN*	(CH <sub>3</sub> ) <sub>3</sub> N···Ag–I	D. Bittner, S. L. Stephens	Spectrum assigned. Manuscript in preparation.
C <sub>3</sub> H <sub>9</sub> F <sub>6</sub> NS*	(CH <sub>3</sub> ) <sub>3</sub> N···SF <sub>6</sub>	D. Bittner	Spectrum assigned.
C <sub>4</sub> H <sub>6</sub> O	(CH <sub>2</sub> ) <sub>2</sub> O···HC≡CH	S. Batten	All singly substituted <sup>13</sup> C species assigned.
C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O*	Urea···imidazole	S. Blanco (Valladolid), J. C. Mullaney, C. Medcraft	Spectrum assigned, isotopic work.
C <sub>4</sub> H <sub>9</sub> NOS*	(CH <sub>3</sub> ) <sub>3</sub> N···S=C=O	E. Gougoula, J. A. Moxon	Published: <i>Molecules</i> , <b>24</b> , 4257, (2019).
C <sub>4</sub> H <sub>9</sub> NS <sub>2</sub> *	(CH <sub>3</sub> ) <sub>3</sub> N···S=C=S	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
FIPt*	FPtI	D. Bittner, G. Cooper, C. Medcraft	Spectra of isotopologues assigned.
H <sub>3</sub> IS	H <sub>2</sub> 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 <sub>3</sub> H <sub>2</sub> O <sub>5</sub> S (HC≡C-COOSO <sub>2</sub> OH)	Propiolic sulfuric anhydride	C.J. Smith A. K. Huff R.M. Ward K.R. Leopold	<i>J. Phys. Chem. A</i> <b>2020</b> , 124, 601. DOI: 10.1021/acs.jpca.9b09310 (Includes review of carboxylic sulfuric anhydrides).
C <sub>2</sub> H <sub>4</sub> OS (CH <sub>3</sub> COSH)	Thioacetic Acid	C.J. Smith A. K. Huff H. Zhang Y. Mo K.R. Leopold	<i>J. Chem. Phys.</i> , <b>2019</b> , 150, 134302. DOI: 10.1063/1.5087718 Internal rotation in two conformers.
C <sub>2</sub> HF <sub>3</sub> O <sub>5</sub> S (CF <sub>3</sub> COOSO <sub>2</sub> OH)	Trifluoroacetic Sulfuric Anhydride	A.K. Huff R.B. Mackenzie C.J. Smith K.R. Leopold	<i>J. Phys. Chem. A</i> , <b>2019</b> , 123, 2237. DOI: 10.1021/acs.jpca.9b00300
C <sub>4</sub> F <sub>6</sub> O <sub>3</sub> (CF <sub>3</sub> COOCOCF <sub>3</sub> )	Trifluoroacetic Anhydride	N. Love C.J. Smith A.K. Huff K.R. Leopold	<i>J. Mol. Spectrosc.</i> <b>2019</b> , 365, 111210.
C <sub>10</sub> H <sub>18</sub> O <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> CCOOCOC(CH <sub>3</sub> ) <sub>3</sub>	Pivalic Anhydride	N. Love A.K. Huff K.R. Leopold	Submitted, <i>J. Mol. Spectrosc.</i> 8 Isotopologues; Description of DAPPERS spectral assignment program.
O <sub>5</sub> S <sub>2</sub> SO <sub>3</sub> -SO <sub>2</sub>	SO <sub>3</sub> -SO <sub>2</sub> complex	A.K. Huff R.M. Ward K.R. Leopold	5 Isotopologues; Manuscript in preparation.
C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> S (CH <sub>3</sub> COSH-H <sub>2</sub> O)	Thioacetic acid – water complex	A.K. Huff C.J. Smith K.R. Leopold	Three isotopologues; Manuscript in preparation.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CHF <sub>3</sub> O <sub>3</sub> S CF <sub>3</sub> SO <sub>2</sub> OH	Triflic Acid	A.K. Huff C.J. Smith N. Love K. R. Leopold	Parent, <sup>34</sup> S, D isotopologues; Tunneling states observed; Manuscript in preparation.
CH <sub>3</sub> F <sub>3</sub> O <sub>4</sub> S CF <sub>3</sub> SO <sub>2</sub> OH-H <sub>2</sub> O	Triflic acid – water complex	A.K. Huff K.R. Leopold	Parent, <sup>34</sup> S, D <sub>2</sub> O, DOH; Tunneling states observed; Manuscript in preparation.
CH <sub>5</sub> F <sub>3</sub> O <sub>5</sub> S CF <sub>3</sub> SO <sub>2</sub> OH-(H <sub>2</sub> O) <sub>2</sub>	Triflic acid – (H <sub>2</sub> O) <sub>2</sub> Complex	A.K. Huff K.R. Leopold	Parent; <sup>34</sup> S; (D <sub>2</sub> O) <sub>2</sub> .
CH <sub>7</sub> F <sub>3</sub> O <sub>6</sub> S CF <sub>3</sub> SO <sub>2</sub> OH-(H <sub>2</sub> O) <sub>3</sub>	Triflic acid – (H <sub>2</sub> O) <sub>3</sub> Complex	A.K. Huff K.R. Leopold	Spectrum assigned and fit.
C <sub>4</sub> H <sub>10</sub> F <sub>3</sub> NO <sub>3</sub> S (CH <sub>3</sub> ) <sub>3</sub> NH <sup>+</sup> -CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup>	Trimethylammonium Triflate Ion Pair	N. Love A.K. Huff K.R. Leopold	Spectrum assigned and fit.
CH <sub>4</sub> O <sub>3</sub> S (CH <sub>3</sub> SO <sub>2</sub> OH)	Methanesulfonic Acid	A.K. Huff N. Love K.R. Leopold	3 Isotopologues; Tunneling states.
CH <sub>6</sub> O <sub>4</sub> S (CH <sub>3</sub> SO <sub>2</sub> OH-H <sub>2</sub> O)	Methanesulfonic Acid – H <sub>2</sub> O Complex	A.K. Huff N. Love K.R. Leopold	Parent, D <sub>2</sub> O, d-MSA-D <sub>2</sub> O complex.
C <sub>4</sub> H <sub>2</sub> F <sub>6</sub> O <sub>4</sub> CF <sub>3</sub> COOCOCF <sub>3</sub> -H <sub>2</sub> O	Trifluoroacetic Anhydride – Water Complex	N. Love A.K. Huff K.R. Leopold	Parent, D <sub>2</sub> O and HDO assigned and fit.
C <sub>7</sub> H <sub>9</sub> F <sub>3</sub> O <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> CCOOCOCF <sub>3</sub>	Pivalic Trifluoro- Acetic Anhydride	N. Love A.K. Huff K.R. Leopold	10 Isotopologues;
C <sub>6</sub> H <sub>11</sub> F <sub>3</sub> O <sub>4</sub> (CH <sub>3</sub> ) <sub>3</sub> CCOOCOCF <sub>3</sub> -H <sub>2</sub> O	Pivalic Trifluoro- Acetic Anhydride- H <sub>2</sub> O Complex	N. Love A.K. Huff K.R. Leopold	Parent assigned and fit; 2 states.
C <sub>10</sub> H <sub>20</sub> O <sub>4</sub> (CH <sub>3</sub> ) <sub>3</sub> CCOOCOC(CH <sub>3</sub> ) <sub>3</sub> - H <sub>2</sub> O	Pivalic Anhydride – Water Complex	N. Love A.K. Huff K.R. Leopold	Parent assigned and fit; 2 states.
C <sub>9</sub> H <sub>5</sub> F <sub>3</sub> O <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COOCOCF <sub>3</sub>	Benzoic Trifluoro- Acetic Anhydride	N. Love A.K. Huff M.A Dvorak K.R. Leopold	Parent assigned and one <sup>13</sup> C isotopologue fit.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> CCOOH	Pivalic Acid	A.K. Huff N. Love K.R. Leopold	Parent assigned and fit.
C <sub>5</sub> H <sub>7</sub> NO (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 <sub>7</sub> H <sub>5</sub> F <sub>2</sub> N (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 <sub>6</sub> H <sub>5</sub> NS <sub>2</sub> (pyridine-CS <sub>2</sub> )	C <sub>5</sub> H <sub>5</sub> N-CS <sub>2</sub> (pyridine-CS <sub>2</sub> complex)	B. Timp, S. Iyer, K.R. Leopold	Spectra observed.
C <sub>3</sub> H <sub>9</sub> ArNO <sub>3</sub> S	(CH <sub>3</sub> ) <sub>3</sub> N-SO <sub>3</sub> -Ar complex	C.T. Dewberry R.B. Mackenzie B.A. Timp K.R. Leopold	Spectra observed.
ArHNO <sub>3</sub> (HNO <sub>3</sub> -Ar)	Nitric acid – Argon complex	J.L. Doran G. Sedo K.R. Leopold	Spectrum observed, rotational assignments.
C <sub>5</sub> H <sub>11</sub> N <sub>3</sub> ((CH <sub>3</sub> ) <sub>3</sub> N-HCN-HCN)	(CH <sub>3</sub> ) <sub>3</sub> N-HCN-HCN complex	M. Craddock C.S. Brauer K.R. Leopold	11 isotopologues assigned and analyzed.
C <sub>3</sub> H <sub>11</sub> F <sub>2</sub> N ((CH <sub>3</sub> ) <sub>3</sub> N-HF-HF)	(CH <sub>3</sub> ) <sub>3</sub> N-HF-HF complex	C.S. Brauer M. Craddock G. Sedo S. W. Hunt K.R. Leopold	8 isotopologues assigned and analyzed Manuscript in preparation.
C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> (CO <sub>2</sub> -C <sub>6</sub> H <sub>6</sub> )	CO <sub>2</sub> -Benzene complex	J.L. Doran K.R. Leopold	Spectrum observed; not assigned.
BF <sub>3</sub> H <sub>2</sub> O (H <sub>2</sub> O-BF <sub>3</sub> )	H <sub>2</sub> O-BF <sub>3</sub> complex	D.L. Fiacco S.W. Hunt K. J. Higgins M.E. Ott K.R. Leopold	6 isotopologues observed; Internal motion
CH <sub>3</sub> BF <sub>4</sub> (CH <sub>3</sub> F-BF <sub>3</sub> )	methyl fluoride-BF <sub>3</sub> complex	J.A. Phillips M. Canagaratna M.E. Ott K.R. Leopold	Spectra observed for <sup>10</sup> B and <sup>11</sup> B species with CH <sub>3</sub> F and <sup>13</sup> CH <sub>3</sub> F; two internal rotor states.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>18</sub> GaN N(CH <sub>3</sub> ) <sub>3</sub> complex	(CH <sub>3</sub> ) <sub>3</sub> Ga-N(CH <sub>3</sub> ) <sub>3</sub>	S.W. Hunt D.L. Fiacco K.R. Leopold	<sup>14</sup> N and <sup>15</sup> N species (CH <sub>3</sub> ) <sub>3</sub> Ga- observed.
ClH <sub>2</sub> NO <sub>3</sub> (HCl-HNO <sub>3</sub> )	HCl-nitric acid complex	M.E. Ott K.R. Leopold	a-type spectrum for <sup>35</sup> Cl, <sup>37</sup> Cl, <sup>14</sup> N, and <sup>15</sup> N and DNO <sub>3</sub> species.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
H <sub>8</sub> OS <sub>3</sub> (H <sub>2</sub> S) <sub>3</sub> ⋯ (H <sub>2</sub> O)	Water ⋯ Hydrogen sulfide complexes	Saragi, Pérez, <sup>a</sup> Schnell, <sup>a</sup> Lesarri	Assigned
H <sub>12</sub> O <sub>3</sub> S <sub>3</sub> (H <sub>2</sub> S) <sub>3</sub> ⋯ (H <sub>2</sub> O) <sub>3</sub>	Water ⋯ Hydrogen sulfide complexes	Saragi, Pérez, <sup>a</sup> Schnell, <sup>a</sup> Lesarri	Assigned
C <sub>2</sub> H <sub>3</sub> OF <sub>5</sub> (CF <sub>3</sub> CF <sub>2</sub> H ⋯ H <sub>2</sub> O)	Pentafluoroethane ⋯ Water	Gou, <sup>b</sup> Feng, <sup>b</sup> Caminati, <sup>c</sup> Grabow, <sup>d</sup> Lesarri	Manuscript
C <sub>4</sub> H <sub>6</sub> F <sub>4</sub> S <sub>3</sub> (C <sub>2</sub> F <sub>4</sub> S <sub>2</sub> ⋯ C <sub>2</sub> H <sub>6</sub> S)	2,2,4,4-Tetrafluoro- 1,3-dithiethane ⋯ Dimethylsulfide	Obenchain, <sup>a,d</sup> Juanes, Spada, <sup>e</sup> Grabow, <sup>b</sup> Lesarri	Assigned
C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>	1,2-Butanedithiol	Juanes, Lesarri	<i>JMS</i> , 2020, in press
C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>	2,3-Butanedithiol	Juanes, Lesarri	Assigned
C <sub>4</sub> H <sub>12</sub> OS (CH <sub>3</sub> CH <sub>2</sub> OH-CH <sub>3</sub> CH <sub>2</sub> SH)	Ethanol ⋯ Ethanethiol	Jin, <sup>b</sup> Zhang, <sup>b</sup> Li, <sup>b</sup> Gou, <sup>b</sup> Feng, <sup>b</sup> Lesarri	Assigned
C <sub>4</sub> H <sub>12</sub> S <sub>2</sub> (CH <sub>3</sub> CH <sub>2</sub> SH) <sub>2</sub>	Ethanethiol dimer	Jin, <sup>b</sup> Zhang, <sup>b</sup> Li, <sup>b</sup> Gou, <sup>b</sup> Feng, <sup>b</sup> Lesarri	Assigned
C <sub>4</sub> H <sub>5</sub> F <sub>3</sub> O <sub>2</sub>	1,1,1-trifluoroacetone ⋯ Formaldehyde	Jin, <sup>b</sup> Gou, <sup>b</sup> Feng, <sup>b</sup> Lesarri	Assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>5</sub> NOS (C <sub>3</sub> H <sub>3</sub> NS ... H <sub>2</sub> CO)	Thiazole ... Formaldehyde	Li, <sup>b</sup> Chen, <sup>b</sup> Feng, <sup>b</sup> Gou, <sup>b</sup> Lesarri	Assigned
C <sub>5</sub> H <sub>6</sub> OS	Thenyl alcohol	Juanes, Saragi, Lesarri	<i>PCCP</i> , 2020, in press
C <sub>5</sub> H <sub>6</sub> S <sub>2</sub>	Thenyl mercaptan	Juanes, Saragi, Lesarri	<i>PCCP</i> , 2020, in press
C <sub>5</sub> H <sub>7</sub> NO	Furfuryl amine	Juanes, Lesarri	Assigned
C <sub>5</sub> H <sub>7</sub> NS	Thenyl amine	Juanes, Lesarri	Assigned
C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> S (C <sub>5</sub> H <sub>6</sub> OS ... H <sub>2</sub> O)	Thenyl alcohol ... Water	Juanes, Saragi, Lesarri	<i>PCCP</i> , 2020, in press
C <sub>5</sub> H <sub>8</sub> OS <sub>2</sub> (C <sub>5</sub> H <sub>6</sub> S <sub>2</sub> ... H <sub>2</sub> O)	Thenyl mercaptan ... Water	Juanes, Saragi, Lesarri	<i>PCCP</i> , 2020, in press,
C <sub>5</sub> H <sub>5</sub> F <sub>3</sub> O <sub>2</sub> (C <sub>4</sub> H <sub>3</sub> F <sub>3</sub> O ... H <sub>2</sub> C=O)	Trifluoroacetone... Formaldehyde	Pérez, <sup>a</sup> Lesarri, Jahn, <sup>d</sup> Dewald, <sup>d</sup> Grabow <sup>d</sup>	Analysis in progress
C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	Lyxose	Calabrese, <sup>f</sup> Écija, <sup>f</sup> Lesarri, Cocinero <sup>f</sup>	<i>JPCL</i> , 2019, 10, 3339
C <sub>6</sub> H <sub>6</sub> OS	3-Mercaptophenol	Juanes, Lesarri	Assigned
C <sub>6</sub> H <sub>7</sub> NS	3-Mercaptoaniline	Juanes, Lesarri	Assigned
C <sub>6</sub> H <sub>8</sub> OS	2-Thiopheneethanol	Juanes, Lesarri	Assigned
C <sub>6</sub> H <sub>8</sub> OS	3-Thiopheneethanol	Juanes, Lesarri	Assigned
C <sub>6</sub> H <sub>9</sub> NS	2-Thiopheneethyl- amine	Juanes, Lesarri	Assigned
C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> S (C <sub>6</sub> H <sub>6</sub> OS ... H <sub>2</sub> O)	3-Mercaptophenol ... Water	Juanes, Lesarri	Assigned
C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> S (C <sub>6</sub> H <sub>8</sub> OS ... H <sub>2</sub> O)	2-Thiopheneethanol ... Water	Juanes, Lesarri	Assigned
C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> S (C <sub>6</sub> H <sub>8</sub> OS ... H <sub>2</sub> O)	3-Thiopheneethanol ... Water	Juanes, Lesarri	Assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>2</sub> F <sub>5</sub> NO (C <sub>5</sub> F <sub>5</sub> N ... H <sub>2</sub> C=O)	Pentafluoropyridine ... Formaldehyde	Gou, <sup>b</sup> Feng, <sup>b</sup> Juanes, Lesarri	Spectrum recorded
C <sub>6</sub> H <sub>12</sub> S	Cyclohexanethiol	Juanes, Lesarri, Evangelisti, <sup>c</sup>	Assigned
C <sub>6</sub> H <sub>13</sub> N	Cyclohexylamine	Juanes, Lesarri	Assigned
C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> S (C <sub>6</sub> H <sub>12</sub> S ... H <sub>2</sub> O)	Cyclohexanethiol ... Water	Juanes, Lesarri, Evangelisti <sup>c</sup>	Assigned
C <sub>6</sub> H <sub>15</sub> NO (C <sub>6</sub> H <sub>13</sub> N ... H <sub>2</sub> O)	Cyclohexylamine ... Water	Juanes, Lesarri,	Assigned
C <sub>6</sub> H <sub>10</sub> S <sub>2</sub>	Diallyl disulfide	Demaison, <sup>g</sup> Vogt, <sup>g</sup> Saragi Juanes, Lesarri,	<i>PCCP</i> , 2019, 21, 19732
C <sub>6</sub> H <sub>11</sub> NO	ε-Caprolactam	Wachsmuth, <sup>d</sup> Vallejo, Lesarri, Grabow <sup>d</sup>	Assigned
C <sub>6</sub> H <sub>12</sub> O	Oxepane	Borter, <sup>d</sup> Wachsmuth, <sup>d</sup> Lesarri, Cocinero, <sup>f</sup> Grabow <sup>d</sup>	Assigned
C <sub>6</sub> H <sub>13</sub> N	Azepane	Wachsmuth, <sup>d</sup> Vallejo, Grabow, <sup>d</sup> Lesarri,	Assigned
C <sub>7</sub> H <sub>8</sub> S	Benzyl mercaptan	Saragi, Juanes, Caminati, <sup>c</sup> Lesarri	<i>JPCA</i> , 2019, 123, 8435
C <sub>7</sub> H <sub>14</sub> S	Cyclohexyl- methanethiol	Jin, <sup>b</sup> Saragi, Feng, <sup>b</sup> Gou, <sup>b</sup> Lesarri	Assigned
C <sub>7</sub> H <sub>10</sub> O <sub>2</sub> (C <sub>7</sub> H <sub>8</sub> O ... H <sub>2</sub> O)	Benzyl alcohol ... Water	Saragi, Lesarri	Assigned
C <sub>7</sub> H <sub>12</sub> O <sub>3</sub> (C <sub>7</sub> H <sub>8</sub> O ... 2 H <sub>2</sub> O)	Benzyl alcohol ... (Water) <sub>2</sub>	Saragi, Lesarri	Assigned
C <sub>7</sub> H <sub>10</sub> OS (C <sub>7</sub> H <sub>8</sub> S ... H <sub>2</sub> O)	Benzyl mercaptan ... Water	Saragi, Lesarri	Assigned
C <sub>7</sub> H <sub>15</sub> NO <sub>2</sub>	4-Amino-2-propyl tetrahydrofuran-3-ol	Saragi, Lesarri	Assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>7</sub> H <sub>17</sub> NO <sub>3</sub> (C <sub>7</sub> H <sub>15</sub> NO <sub>2</sub> ... H <sub>2</sub> O)	4-amino-2-propyl tetrahydrofuran-3-ol ... Water	Saragi, Lesarri	Assigned
C <sub>8</sub> H <sub>10</sub> O	1-Phenylethanol	Juanes, Saragi, Lesarri	Assigned
C <sub>8</sub> H <sub>10</sub> S	Phenylethyl mercaptan	Saragi, Lesarri	Assigned
C <sub>8</sub> H <sub>16</sub> O	Cyclohexyl ethanol	Jin, <sup>b</sup> Saragi, Gang, <sup>b</sup> Gou, <sup>b</sup> Lesarri	Assigned
C <sub>8</sub> H <sub>11</sub> N	1-Phenylethylamine	Saragi, Juanes, Lesarri	Assigned
C <sub>8</sub> H <sub>12</sub> N	Cyanocycloheptane	Wachsmuth, <sup>d</sup> Lesarri Grabow <sup>d</sup>	In preparation
C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> (C <sub>4</sub> H <sub>8</sub> O) <sub>2</sub>	Tetrahydrofuran dimer	Saragi, Pérez, <sup>a</sup> Schnell, <sup>a</sup> Lesarri	Assigned
C <sub>8</sub> H <sub>12</sub> O <sub>2</sub> (C <sub>8</sub> H <sub>10</sub> O ... H <sub>2</sub> O)	Phenylethyl alcohol ... Water	Saragi, Lesarri	Assigned
C <sub>8</sub> H <sub>12</sub> OS (C <sub>8</sub> H <sub>10</sub> S ... H <sub>2</sub> O)	Phenylethyl mercaptan ... Water	Saragi, Lesarri	Assigned
C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>	1,7-dioxaspiro[5.5]undecane	Saragi, Juanes, Lesarri	Assigned
C <sub>9</sub> H <sub>13</sub> NO <sub>3</sub> (C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub> ...H <sub>2</sub> O)	Benzocaine ... Water	Lesarri, Shipman, <sup>h</sup> Pate <sup>i</sup>	Assigned
C <sub>10</sub> H <sub>12</sub> O <sub>4</sub> (C <sub>5</sub> H <sub>6</sub> O <sub>2</sub> ) <sub>2</sub>	Furfuryl alcohol dimer	Juanes, Saragi, Lesarri	Assigned
C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> S <sub>2</sub> (C <sub>5</sub> H <sub>6</sub> OS) <sub>2</sub>	Thenyl alcohol dimer	Juanes, Saragi, Lesarri	Assigned
C <sub>10</sub> H <sub>16</sub> O	2-adamantanol	Juanes, Saragi, Lesarri	Assigned
C <sub>10</sub> H <sub>18</sub> O <sub>2</sub> (C <sub>10</sub> H <sub>16</sub> O ... H <sub>2</sub> O)	2-adamantanol ... Water	Juanes, Saragi, Lesarri	Assigned



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>10</sub> H <sub>12</sub> O <sub>3</sub> (HO C <sub>6</sub> H <sub>3</sub> (OCH <sub>3</sub> )C <sub>2</sub> H <sub>2</sub> CH <sub>2</sub> OH)	Coniferyl alcohol	Cocinero, <sup>f</sup> Lesarri	In preparation
C <sub>10</sub> H <sub>14</sub> O <sub>3</sub> (HO C <sub>6</sub> H <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CO)CH <sub>3</sub> )	Zingerone	Cocinero, <sup>f</sup> Lesarri, Caminati <sup>b</sup>	In preparation
C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub> (NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> COO(CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub> )	Butamben	Caminati, <sup>c</sup> Grabow <sup>d</sup> Lesarri, Cocinero, <sup>f</sup>	<i>ChemComm</i> , 2020, in press
C <sub>11</sub> H <sub>15</sub> NO <sub>2</sub> (NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> COOCH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> )	Isobutamben	Caminati, <sup>c</sup> Grabow <sup>d</sup> Lesarri, Cocinero, <sup>f</sup>	ChemComm 2020, in press
C <sub>12</sub> H <sub>22</sub> S <sub>2</sub>	Dicyclohexyl disulfide	Saragi, Lesarri	Assigned
C <sub>12</sub> H <sub>12</sub> S <sub>2</sub> (C <sub>6</sub> H <sub>6</sub> S) <sub>2</sub>	Thiophenol dimer	Saragi, Juanes, Pérez, <sup>a</sup> Schnell, <sup>a</sup> Lesarri	In preparation
C <sub>12</sub> H <sub>24</sub> O <sub>3</sub>	Tetrahydrofuran trimer	Saragi, Pérez, <sup>a</sup> Schnell, <sup>a</sup> Lesarri	Assigned
C <sub>12</sub> H <sub>16</sub> O <sub>2</sub> S <sub>2</sub> (C <sub>6</sub> H <sub>8</sub> OS) <sub>2</sub>	2-Thiopheneethanol Dimer	Juanes, Lesarri	Assigned
C <sub>12</sub> H <sub>16</sub> O <sub>2</sub> S <sub>2</sub> (C <sub>6</sub> H <sub>8</sub> OS) <sub>2</sub>	3-Thiopheneethanol Dimer	Juanes, Lesarri	Assigned
C <sub>12</sub> H <sub>24</sub> O <sub>2</sub> (C <sub>6</sub> H <sub>12</sub> O) <sub>2</sub>	Cyclohexanol dimer	Juanes, Usabiaga, <sup>f</sup> León, Evangelisti, <sup>c</sup> Lesarri	Submitted
C <sub>12</sub> H <sub>26</sub> N <sub>2</sub> (C <sub>6</sub> H <sub>13</sub> N) <sub>2</sub>	Cyclohexyl amine dimer	Juanes, Lesarri	Assigned
C <sub>12</sub> H <sub>10</sub> S <sub>2</sub>	Diphenyl disulfide	Demaison, <sup>g</sup> Vogt, <sup>g</sup> Saragi, Juanes, Rudolph, <sup>g</sup> Lesarri	<i>CPC</i> , 2019, 20, 366
C <sub>12</sub> H <sub>22</sub> S <sub>2</sub>	Dicyclohexyl disulfide	Saragi, Juanes, Lesarri	Assigned
C <sub>13</sub> H <sub>11</sub> O <sub>4</sub> P	Phenyl saligenin phosphate	Juanes, Saragi, Lesarri	<i>PCCP</i> , 2019, 21, 16418
C <sub>14</sub> H <sub>13</sub> O <sub>4</sub> P	Cresyl saligenin phosphate	Juanes, Saragi, Lesarri	<i>PCCP</i> , 2019, 21, 16418

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>14</sub> H <sub>16</sub> O <sub>2</sub> (C <sub>7</sub> H <sub>8</sub> O) <sub>2</sub>	Benzyl alcohol dimer	Saragi, Lesarri	Assigned
C <sub>14</sub> H <sub>16</sub> S <sub>2</sub> (C <sub>7</sub> H <sub>8</sub> S) <sub>2</sub>	Benzyl mercaptan dimer	Saragi, Lesarri	Assigned
C <sub>14</sub> H <sub>28</sub> S <sub>2</sub> (C <sub>7</sub> H <sub>14</sub> S) <sub>2</sub>	Cyclohexyl-methanethiol dimer	Jin, <sup>b</sup> Saragi, Feng, <sup>b</sup> Gou, <sup>b</sup> Lesarri	Assigned
C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O	Matrine	Juanes, Saragi, Lesarri	Submitted
C <sub>16</sub> H <sub>20</sub> O <sub>2</sub> (C <sub>8</sub> H <sub>10</sub> O) <sub>2</sub>	Phenylethyl alcohol dimer	Saragi, Lesarri	Assigned
C <sub>16</sub> H <sub>20</sub> O <sub>2</sub> (C <sub>8</sub> H <sub>10</sub> O) <sub>2</sub>	1-Phenylethanol dimer	Juanes, Lesarri	Assigned
C <sub>16</sub> H <sub>20</sub> S <sub>2</sub> (C <sub>8</sub> H <sub>10</sub> S) <sub>2</sub>	Phenylethyl mercaptan dimer	Saragi, Lesarri	Assigned
C <sub>16</sub> H <sub>32</sub> O <sub>2</sub> (C <sub>8</sub> H <sub>16</sub> O) <sub>2</sub>	Cyclohexyl ethanol dimer	Jin, <sup>b</sup> Saragi, Feng, <sup>b</sup> Gou, <sup>b</sup> Lesarri	Assigned
C <sub>20</sub> H <sub>32</sub> O <sub>2</sub> (C <sub>10</sub> H <sub>16</sub> O) <sub>2</sub>	2-adamantanol dimer	Juanes, Saragi, Lesarri	Assigned

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
C <sub>2</sub> HClF <sub>2</sub> ( <i>E</i> )-CF <sup>35</sup> CiCHF, ( <i>E</i> )-CF <sup>37</sup> CiCHF, ( <i>E</i> )- <sup>13</sup> CF <sup>35</sup> CiCHF, ( <i>E</i> )-CF <sup>35</sup> Cl <sup>13</sup> CHF)	( <i>E</i> )-1-chloro- 1,2-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.
C <sub>2</sub> H <sub>2</sub> ClF <sub>3</sub> (HF-( <i>E</i> )-CF <sup>35</sup> CiCHF, HF-( <i>E</i> )-CF <sup>37</sup> CiCHF, DF-( <i>E</i> )-CF <sup>35</sup> CiCHF, DF-( <i>E</i> )-CF <sup>37</sup> CiCHF)	hydrogen fluoride- ( <i>E</i> )-1-chloro- 1,2-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.
C <sub>4</sub> H <sub>3</sub> ClF <sub>2</sub> (HCCH-( <i>E</i> )-CF <sup>35</sup> CiCHF, HCCH-( <i>E</i> )-CF <sup>37</sup> CiCHF, H <sup>13</sup> CCH-( <i>E</i> )-CF <sup>35</sup> CiCHF, HC <sup>13</sup> CH-( <i>E</i> )-CF <sup>35</sup> CiCHF)	acetylene- ( <i>E</i> )-1-chloro- 1,2-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned. Manuscript in prep.
C <sub>2</sub> HArClF <sub>2</sub> (Ar-( <i>E</i> )-CF <sup>35</sup> CiCHF, Ar-( <i>E</i> )-CF <sup>37</sup> CiCHF, Ar-( <i>E</i> )- <sup>13</sup> CF <sup>35</sup> CiCHF, Ar-( <i>E</i> )-CF <sup>35</sup> Cl <sup>13</sup> CHF)	argon-( <i>E</i> )-1-chloro- 1,2-difluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>2</sub> H <sub>3</sub> ClF <sub>2</sub> (H <sup>35</sup> Cl- <i>cis</i> -CHFCHF, H <sup>37</sup> Cl- <i>cis</i> -CHFCHF, H <sup>35</sup> Cl- <i>cis</i> - <sup>13</sup> 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 <sub>4</sub> H <sub>4</sub> F <sub>2</sub> (HCCH- <i>cis</i> -CHFCHF, H <sup>13</sup> CCH- <i>cis</i> -CHFCHF, HC <sup>13</sup> CH- <i>cis</i> -CHFCHF, HCCH- <i>cis</i> - <sup>13</sup> CHFCHF, HCCH- <i>cis</i> -CHF <sup>13</sup> CHF)	acetylene- <i>cis</i> -1,2-difluoro- ethylene	Helen O. Leung Mark D. Marshall	J. Chem. Phys. 152, 034303 (2020)
C <sub>4</sub> H <sub>3</sub> ClF <sub>2</sub> (HCCH-CF <sub>2</sub> CH <sup>35</sup> Cl, HCCH-CF <sub>2</sub> CH <sup>37</sup> Cl, H <sup>13</sup> CCH-CF <sub>2</sub> CH <sup>35</sup> Cl, HC <sup>13</sup> CH-CF <sub>2</sub> CH <sup>35</sup> Cl)	acetylene-2-chloro- 1,1-difluoroethylene	Helen O. Leung Mark D. Marshall	J. Phys. Chem. A <b>124</b> , 1382 (2020)
C <sub>2</sub> H <sub>2</sub> DF <sub>3</sub> (DF- <i>cis</i> -CHFCHF, DF- <i>cis</i> - <sup>13</sup> CHFCHF, DF- <i>cis</i> -CHF <sup>13</sup> CHF)	deuterium fluoride- <i>cis</i> -1,2-difluoro- ethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>2</sub> H <sub>3</sub> ArCl (Ar-CH <sub>2</sub> CH <sup>35</sup> Cl, Ar-CH <sub>2</sub> CH <sup>37</sup> Cl)	argon-vinyl chloride	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> (H <sup>35</sup> Cl-CH <sub>2</sub> CH <sup>35</sup> Cl, H <sup>35</sup> Cl-CH <sub>2</sub> CH <sup>37</sup> Cl, H <sup>37</sup> Cl-CH <sub>2</sub> CH <sup>35</sup> Cl)	hydrogen chloride- vinyl chloride	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>2</sub> H <sub>3</sub> Cl <sub>2</sub> F (H <sup>35</sup> Cl-( <i>Z</i> )-CHFCH <sup>35</sup> Cl, H <sup>37</sup> Cl-( <i>Z</i> )-CHFCH <sup>35</sup> Cl, H <sup>35</sup> Cl-( <i>Z</i> )-CHFCH <sup>37</sup> Cl)	hydrogen chloride- ( <i>Z</i> )-1-chloro-2- fluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>2</sub> H <sub>2</sub> ArClF (Ar-CH <sub>2</sub> CF <sup>35</sup> Cl, Ar-CH <sub>2</sub> CF <sup>37</sup> Cl)	argon-1-chloro- 1-fluoroethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>2</sub> H <sub>3</sub> Cl <sub>2</sub> F (H <sup>35</sup> Cl-CH <sub>2</sub> CF <sup>35</sup> Cl, H <sup>35</sup> Cl-CH <sub>2</sub> CF <sup>37</sup> Cl, H <sup>37</sup> Cl-CH <sub>2</sub> CF <sup>35</sup> Cl)	hydrogen chloride- 1-chloro-1-fluoro- ethylene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> (CH <sup>35</sup> ClCH <sup>35</sup> Cl, CH <sup>35</sup> ClCH <sup>37</sup> Cl, CH <sup>37</sup> ClCH <sup>37</sup> Cl, CH <sup>35</sup> Cl <sup>13</sup> CH <sup>35</sup> 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.
$C_6H_6F_6O_2$ ( $CH_2CH(CF_3)O-CH_2CH(CF_3)O$ )	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. Manuscript in prep.
$C_3H_5FO$ ( $CH_2CH(CFH_2)O$ , $^{13}CH_2CH(CFH_2)O$ , $CH_2^{13}CH(CFH_2)O$ , $CH_2CH(^{13}CFH_2)O$ , $CH_2CH(CFH_2)^{18}O$ )	2-(fluoromethyl)-oxirane	Helen O. Leung Mark D. Marshall	J. Phys. Chem. A <b>124</b> , 1798 (2020)
$C_3H_5ArFO$ ( $Ar-CH_2CH(CFH_2)O$ )	argon-2-(fluoromethyl)-oxirane	Helen O. Leung Mark D. Marshall	J. Phys. Chem. A <b>124</b> , 1798 (2020)
$C_3H_2F_4O$ ( <i>cis</i> -CHFCH(CF <sub>3</sub> )O, <i>cis</i> - <sup>13</sup> CHFCH(CF <sub>3</sub> )O, <i>cis</i> -CHF <sup>13</sup> CH(CF <sub>3</sub> )O, <i>cis</i> -CHFCH(CF <sub>3</sub> ) <sup>18</sup> O, <i>cis</i> -CHFCH( <sup>13</sup> CF <sub>3</sub> )O)	<i>cis</i> -1,3,3,3-tetrafluoro-1,2-epoxypropane	Helen O. Leung Mark D. Marshall	Spectrum assigned.
$C_3H_2ArF_4O$ ( <i>cis</i> -CHFCH(CF <sub>3</sub> )O)	argon- <i>cis</i> -1,3,3,3-tetrafluoro-1,2-epoxypropane	Helen O. Leung Mark D. Marshall	Spectrum assigned.

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
C <sub>3</sub> H <sub>2</sub> F <sub>4</sub> O ( <i>trans</i> -CHFCH(CF <sub>3</sub> )O, <i>trans</i> - <sup>13</sup> CHFCH(CF <sub>3</sub> )O, <i>trans</i> -CHF <sup>13</sup> CH(CF <sub>3</sub> )O, <i>trans</i> -CHFCH(CF <sub>3</sub> ) <sup>18</sup> O, <i>trans</i> -CHFCH( <sup>13</sup> CF <sub>3</sub> )O)	<i>trans</i> -1,3,3,3-tetrafluoro-1,2-epoxypropane	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>3</sub> H <sub>2</sub> ArF <sub>4</sub> O (Ar- <i>trans</i> -CHFCH(CF <sub>3</sub> )O)	argon- <i>trans</i> -1,3,3,3-tetrafluoro-1,2-epoxypropane	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>3</sub> H <sub>6</sub> ArO <sub>2</sub> (Ar-CH <sub>2</sub> CH(CH <sub>2</sub> OH)O)	argon-oxiranylmethanol	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>6</sub> H <sub>10</sub> F <sub>2</sub> O <sub>2</sub> (CH <sub>2</sub> CH(CFH <sub>2</sub> )O-CH <sub>2</sub> CH(CFH <sub>2</sub> )O)	2-(fluoromethyl)-oxirane dimer	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>6</sub> H <sub>10</sub> F <sub>2</sub> O <sub>2</sub> (CH <sub>2</sub> CH(CF <sub>2</sub> H)O-CH <sub>2</sub> CH(CF <sub>2</sub> H)O)	2-(difluoromethyl)-oxirane dimer	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>4</sub> H <sub>6</sub> O (CH <sub>2</sub> CH(CHCH <sub>2</sub> )O, <sup>13</sup> CH <sub>2</sub> CH(CHCH <sub>2</sub> )O, CH <sub>2</sub> <sup>13</sup> CH(CHCH <sub>2</sub> )O, CH <sub>2</sub> CH( <sup>13</sup> CHCH <sub>2</sub> )O, CH <sub>2</sub> CH(CH <sup>13</sup> CH <sub>2</sub> )O, CH <sub>2</sub> CH(CHCH <sub>2</sub> ) <sup>18</sup> O)	2-vinyloxirane	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>4</sub> H <sub>6</sub> ArO (Ar-CH <sub>2</sub> CH(CHCH <sub>2</sub> )O)	argon-2-vinyloxirane	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>3</sub> H <sub>3</sub> ClF <sub>4</sub> (H <sup>35</sup> Cl-CH <sub>2</sub> CFCF <sub>3</sub> )	hydrogen chloride-2,3,3,3-tetrafluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>3</sub> H <sub>2</sub> ClF <sub>3</sub> (CH <sub>2</sub> C <sup>35</sup> ClCF <sub>3</sub> , <sup>13</sup> CH <sub>2</sub> C <sup>35</sup> ClCF <sub>3</sub> , CH <sub>2</sub> <sup>13</sup> C <sup>35</sup> ClCF <sub>3</sub> , CH <sub>2</sub> C <sup>35</sup> Cl <sup>13</sup> CF <sub>3</sub> , CH <sub>2</sub> C <sup>37</sup> ClCF <sub>3</sub> )	2-chloro-3,3,3-trifluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.
C <sub>3</sub> H <sub>2</sub> ArClF <sub>3</sub> (Ar-CH <sub>2</sub> C <sup>35</sup> ClCF <sub>3</sub> , Ar-CH <sub>2</sub> C <sup>37</sup> ClCF <sub>3</sub> )	argon-2-chloro-3,3,3-trifluoropropene	Helen O. Leung Mark D. Marshall	Spectrum assigned.

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

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>5</sub> H <sub>4</sub> F <sub>6</sub> O <sub>4</sub> (HCOOH- (CF <sub>3</sub> ) <sub>2</sub> CHCOOH)	Formic acid-3,3,3- trifluoro-2- (trifluoromethyl)pro panoic acid	Javix Thomas <sup>7</sup> , Michael J. Carrillo, Agapito Serrato III, Fan Xie, Wolfgang Jaeger <sup>7</sup> , Yunjie Xu <sup>7</sup> , Wei Lin	Mol. Phys 117,1193, 2019
C <sub>3</sub> H <sub>2</sub> F <sub>4</sub> O <sub>2</sub> (CF <sub>3</sub> CFHCOOH)	2,3,3,3- tetrafluoropropionic acid	Dan A. Obenchain <sup>1</sup> , Jianming Wu <sup>6</sup> , Xin Xu <sup>6</sup> , Agapito Serrato III, Will Orellana <sup>1</sup> , Stephen A. Cooke <sup>4</sup> , Stewart E. Novick <sup>1</sup> , Wei Lin	To be submitted
C <sub>3</sub> H <sub>4</sub> F <sub>4</sub> O <sub>3</sub> (H <sub>2</sub> O- CF <sub>3</sub> CFHCOOH)	Water-2,3,3,3- tetrafluoropropionic acid	Dan A. Obenchain <sup>1</sup> , Jianming Wu <sup>6</sup> , Xin Xu <sup>6</sup> , Agapito Serrato III, Will Orellana <sup>1</sup> , Stephen A. Cooke <sup>4</sup> , Stewart E. Novick <sup>1</sup> , Wei Lin	To be submitted
C <sub>5</sub> H <sub>8</sub> Ne (Ne- CH <sub>2</sub> =c- CCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> )	Neon-Methylene Cyclobutane	Andrea Minei <sup>2</sup> , Wei Lin, Lu Kang <sup>3</sup> , Wallace C. Pringle <sup>1</sup> , Stewart E. Novick <sup>1</sup>	Manuscript to be submitted
C <sub>2</sub> H <sub>4</sub> I <sub>2</sub>	1,1-diiodoethane	Michael J. Carrillo, Wei Lin, Yasuki Endo <sup>9</sup>	Assignment in progress
C <sub>2</sub> H <sub>4</sub> I	1-Iodoethyl radical (CHI-CH <sub>3</sub> )	Michael J. Carrillo, Wei Lin, Yasuki Endo <sup>9</sup>	Assignment in progress
C <sub>2</sub> H <sub>4</sub> I	2-Iodoethyl radical (CH <sub>2</sub> I-CH <sub>2</sub> )	Michael J. Carrillo, Wei Lin, Yasuki Endo <sup>9</sup>	Assignment in progress
C <sub>2</sub> H <sub>4</sub> Cl	1-Chloroethyl radical (CHCl-CH <sub>3</sub> )	Michael J. Carrillo, Wei Lin, Yasuki Endo <sup>9</sup>	Assignment in progress



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>2</sub> H <sub>4</sub> Cl	2-Chloroethyl radical (CH <sub>2</sub> Cl-CH <sub>2</sub> )	Michael J. Carrillo, Wei Lin, Yasuki Endo <sup>9</sup>	Assignment in progress
C <sub>2</sub> H <sub>4</sub> F	2-Fluoroethyl radical (CH <sub>2</sub> F-CH <sub>2</sub> )	Michael J. Carrillo, Wei Lin, Yasuki Endo <sup>9</sup>	Assignment in progress
C <sub>4</sub> H <sub>3</sub> F <sub>5</sub> O <sub>4</sub> (HCOOH-CF <sub>3</sub> CF <sub>2</sub> COOH)	Formic acid-Pentafluoropropionic acid	Dan A. Obenchain <sup>1</sup> , Stephen A. Cooke <sup>4</sup> , Stewart E. Novick <sup>1</sup> , Wei Lin	Spectrum assigned
C <sub>3</sub> H <sub>10</sub> O (H <sub>2</sub> O-CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub> )	Water propane (C <sup>13</sup> isotopomers)	Dan A. Obenchain <sup>1</sup> , Wei Lin, Karen Peterson <sup>8</sup> , Richard J. Saykally <sup>5</sup> , Stewart E. Novick <sup>1</sup>	Spectrum assigned
C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> (c-CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CHCOOH)	Cyclobutanecarboxylic acid	Michael J. Carrillo, Zunwu Zhou <sup>10</sup> , Shervin Fatehi, Stephen K. Kukolich <sup>10</sup> , 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>
$C_mH_{3m+2n}N_mO_{m+n}$ $(CH_3NO)_m-(H_2O)_n$	formamide-water complexes	Susana Blanco Juan C. López Pablo Pinacho Brooks Pate's Group <sup>1</sup>	Spectra assigned
$C_2H_{5+2n}NO_{2+n}$ $C_2H_5NO_2-(H_2O)_n$	Methyl carbamate (Urethylane) water complexes	Susana Blanco Pablo Pinacho Juan C. López Z. Kisiel <sup>2</sup>	Manuscript in preparation
$C_4H_6O_3$ $(C_3H_4O_2-CH_2O)$	beta-propiolactone-formaldehyde complex	Juan C. López Susana Blanco	Spectrum assigned Work in progress
$C_3H_{5+2n}NO_{1+n}$ $C_3H_5NO-(H_2O)_n$	2-azetidinone-water complexes	Pablo Pinacho Susana Blanco Juan C. López	Spectrum observed Work in progress
$C_3H_{7+2n}NO_{2+n}$ $C_3H_7NO_2-(H_2O)_n$	Ethyl carbamate (Urethane) water complexes	Susana Blanco Pablo Pinacho Juan C. López Z. Kisiel <sup>2</sup>	Manuscript in preparation
$C_5H_{11+2n}NO_{2+n}$ $C_5H_{11}NO_2-(H_2O)_n$	Butyl carbamate water complexes	Susana Blanco Pablo Pinacho Juan C. López Z. Kisiel <sup>2</sup>	<i>J. Phys. Chem. A</i> <i>21, 2177, 2019</i>
$C_5H_{12}O$ $C_5H_{12+2n}O_{1+n}$ $C_5H_{12}ArO$	3-methyl-butanol and water complex and Ar complex	Juan C. López Susana Blanco Alberto Lesarri	Spectra assigned Work in progress
$C_6H_2F_5NO$ $(C_5F_5N-CH_2O)$	Pentafluoropyridine-formaldehyde complex	Alberto Macario Juan C. López Susana Blanco	Spectrum assigned Work in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O (C <sub>5</sub> H <sub>5</sub> N-CH <sub>3</sub> NO)	Pyridine-formamide complex	Susana Blanco Cristina Puzzarini <sup>3</sup> Juan C. López Lorenzo Spada <sup>3</sup>	Spectrum assigned
C <sub>7</sub> H <sub>9</sub> NO (C <sub>5</sub> H <sub>5</sub> N-C <sub>2</sub> H <sub>4</sub> O)	Pyridine-acetaldehyde complex	Susana Blanco Alberto Macario Juan C. López	<i>PCCP 21, 20556, 2019</i>
C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O (C <sub>5</sub> H <sub>5</sub> N-C <sub>2</sub> H <sub>5</sub> NO)	Pyridine-N-Methylformamide complex	Lorenzo Spada <sup>3</sup> Juan C. López Cristina Puzzarini <sup>3</sup> Susana Blanco	Spectrum assigned
C <sub>8</sub> H <sub>11</sub> NO (C <sub>5</sub> H <sub>5</sub> N-C <sub>3</sub> H <sub>6</sub> O)	Pyridine-acetone complex	Juan C. López Susana Blanco	Manuscript in preparation
C <sub>9</sub> H <sub>13</sub> NO (C <sub>5</sub> H <sub>5</sub> N-C <sub>4</sub> H <sub>8</sub> O)	Pyridine-2 butanone complex	Juan C. López Susana Blanco	Manuscript in preparation
C <sub>13</sub> H <sub>11</sub> NO (C <sub>5</sub> H <sub>5</sub> N-C <sub>7</sub> H <sub>6</sub> O)	Pyridine-Benzaldehyde complex	Susana Blanco Juan C. López	Spectrum assigned Work in progress
C <sub>7</sub> H <sub>2</sub> F <sub>6</sub> O (C <sub>6</sub> F <sub>6</sub> -CH <sub>2</sub> O)	Hexafluorobenzene-formaldehyde complex	Susana Blanco Juan C. López Alberto Macario	Spectra assigned Work in progress
C <sub>11</sub> H <sub>5</sub> F <sub>6</sub> N (C <sub>6</sub> F <sub>6</sub> -C <sub>5</sub> H <sub>5</sub> N)	Hexafluorobenzene-pyridine complex	Susana Blanco Juan C. López	Spectra assigned Work in progress
C <sub>7</sub> H <sub>6+2n</sub> O <sub>3+n</sub> C <sub>7</sub> H <sub>6</sub> O <sub>3</sub> -(H <sub>2</sub> O) <sub>n</sub>	Salicylic acid water complexes	Susana Blanco Juan C. López	Manuscript in preparation
C <sub>7</sub> H <sub>7+2n</sub> NO <sub>2+n</sub> C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> -(H <sub>2</sub> O) <sub>n</sub>	Phenyl carbamate water complexes	Pablo Pinacho Susana Blanco Juan C. López	Spectrum observed Work in progress
C <sub>8</sub> H <sub>5</sub> F <sub>5</sub> O (C <sub>7</sub> F <sub>5</sub> H <sub>3</sub> -CH <sub>2</sub> O)	Pentafluorotoluene-formaldehyde complex	Susana Blanco Juan C. López	Spectra assigned Work in progress
C <sub>8</sub> H <sub>10</sub> O <sub>4</sub> C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> -(H <sub>2</sub> O)	o-anisic acid-water complexes	Alberto Macario Susana Blanco Juan C. López	<i>PCCP 21, 6844, 2019</i>
C <sub>9</sub> H <sub>10</sub> O <sub>5</sub> C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> -(CH <sub>2</sub> O <sub>2</sub> )	o-anisic acid – formic acid complexes	Alberto Macario Susana Blanco Juan C. López Yunjie Xu's Group <sup>4</sup>	<i>Chem. Eur. J. 25, 12325, 2019</i>

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> C <sub>9</sub> H <sub>10</sub> O <sub>5</sub>	3-Methoxybenzoic acid ( <i>m</i> -Anisic acid) and formic acid complex	Alberto Macario Susana Blanco Juan C. López Yunjie Xu's Group <sup>4</sup>	<i>J. Phys. Chem. A</i> 123, 6772, 2019
C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> C <sub>8</sub> H <sub>8+2n</sub> O <sub>3+n</sub>	Mandelic acid and water complexes	Pablo Pinacho Susana Blanco Juan C. López	Spectra observed
C <sub>8</sub> H <sub>9+2n</sub> NO <sub>2+n</sub>	Benzyl carbamate water complexes	Pablo Pinacho Juan C. López Susana Blanco	Spectrum observed Work in progress
C <sub>8</sub> H <sub>10</sub> O C <sub>8</sub> H <sub>10+2n</sub> O <sub>1+n</sub>	4-ethylphenol and water complexes	Susana Blanco Juan C. López	Spectra assigned Work in progress
C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> C <sub>8</sub> H <sub>10+2n</sub> O <sub>2+n</sub>	Dimethoxybenzene and water complexes	Assimo Maris <sup>5</sup> Susana Blanco Juan C. López	Spectrum observed
C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>	Caffeine	Susana Blanco Juan C. López	Spectrum observed
C <sub>8</sub> H <sub>17</sub> NO <sub>3</sub>	1-aza-12-crown-4	Susana Blanco Juan C. López	Spectrum assigned Work in progress
C <sub>9</sub> H <sub>10</sub> O <sub>3</sub> C <sub>9</sub> H <sub>10+2n</sub> O <sub>3+n</sub> C <sub>10</sub> H <sub>12</sub> O <sub>5</sub>	Methyl 2-methoxy-benzoate and water complexes and formic acid complexes	Susana Blanco Juan C. López Alberto Macario	Manuscript in preparation
C <sub>9</sub> H <sub>12</sub> O <sub>2</sub> C <sub>9</sub> H <sub>12+2n</sub> O <sub>2+n</sub>	4-Ethylguaiacol and water complexes	Susana Blanco Juan C. López Alberto Macario	Manuscript in preparation
C <sub>9</sub> H <sub>18</sub> O <sub>6</sub>	Triacetone triperoxide (TATP)	Susana Blanco Alberto Macario Juan C. López	Manuscript submitted
C <sub>10</sub> H <sub>8+2n</sub> N <sub>2</sub> O <sub>n</sub>	2,2'-Bipyridine water complex	Susana Blanco Juan C. López Alberto Macario	Spectra assigned Work in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{10}H_{10}O_3$ $C_{10}H_{10+2n}O_{3+n}$	3-Methoxycinnamic acid and water complexes	Alberto Macario Juan C. López Susana Blanco	Spectra observed Work in progress
$C_{10}H_{16}O$ $C_{10}H_{16+2n}O_{1+n}$	Verbenol and water complexes	Assimo Maris <sup>5</sup> Susana Blanco Juan C. López	<i>PCCP, in press.</i> <b>2020</b>
$C_{10}H_{21}NO_4$	1-aza-15-crown-5	Susana Blanco Juan C. López	Spectrum observed
$C_{11}H_9N$ $C_{11}H_{9+2n}NO_n$	2-Phenylpyridine and water complexes	Alberto Macario Juan C. López Susana Blanco	Manuscript in preparation
$C_{11}H_9N$ $C_{11+2n}H_{9+6n}NO_n$	2-Phenylpyridine and ethanol complexes	Alberto Macario Juan C. López Susana Blanco	Spectra assigned Work in progress
$C_{11}H_9N$ $C_{11+n}H_{9+4n}NO_n$	2-Phenylpyridine and methanol complexes	Alberto Macario Juan C. López Susana Blanco	Work in progress
$C_{13}H_{13}NO$	Methoxybiphenyl-amonium	Susana Blanco Juan C. López	Spectrum assigned
$C_{14}H_{20}O_5$	Benzo-5-crown-5 ether	Susana Blanco Juan C. López	Spectra observed Work in progress
$C_{15}H_{10}O_2$ $C_{15}H_{10+2n}O_{2+n}$	Flavone and water complex	Susana Blanco Juan C. López	Spectra assigned Work in progress
$C_{15}H_{12}O_2$ $C_{15}H_{12+2n}O_{2+n}$	Flavanone and water complex	Susana Blanco Juan C. López	Spectra assigned Work in progress

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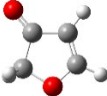
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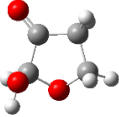
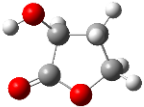
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<sup>a</sup> [https://www.researchgate.net/profile/Francis\\_Lovas/research](https://www.researchgate.net/profile/Francis_Lovas/research)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH <sub>3</sub> N (CH <sub>2</sub> NH)	Methyleneimine	Scherschligt <sup>1</sup> , Douglass <sup>1</sup> , Plusquellic <sup>2</sup> , Lovas <sup>1</sup>	Spectrum measured near 550 GHz
CH <sub>5</sub> N (CH <sub>3</sub> NH <sub>2</sub> )	Methylamine	Scherschligt <sup>1</sup> , Douglass <sup>1</sup> , Plusquellic <sup>2</sup> , Lovas <sup>1</sup>	Spectrum measured 530 to 600 GHz
CH <sub>5</sub> NO <sub>2</sub> (HCOOH-NH <sub>3</sub> )	Formic acid- ammonia	Grabow <sup>3</sup> , Lovas <sup>1</sup> , Fraser <sup>1</sup>	Spectrum assigned For normal species
C <sub>2</sub> H <sub>5</sub> NO (CH <sub>3</sub> OH-HCN)	Methanol-hydrogen cyanide	Lovas <sup>1</sup> , Sobhanadri <sup>4</sup>	Spectrum assigned for 4 isotopomers <b>See Researchgate<sup>a</sup></b>
C <sub>3</sub> H <sub>2</sub> O (HCCCHO)	Propynal	Plusquellic <sup>2</sup> , Lovas <sup>1</sup> , Scherschligt <sup>1</sup> , Douglass <sup>1</sup> ,	mm spectrum assigned
C <sub>3</sub> H <sub>3</sub> F <sub>5</sub> O (CF <sub>3</sub> CH <sub>2</sub> OCHF <sub>2</sub> )	2,2,2-Trifluoroethyl difluoromethyl ether [RE245]	Lovas <sup>1</sup> , Suenram <sup>5</sup> , Hight Walker <sup>1</sup> , Dixon <sup>1,6</sup>	Lowest energy conformer, <i>anti-anti</i> , assigned.
C <sub>3</sub> H <sub>4</sub> O (CH <sub>2</sub> =CHCHO)	Propenal	Plusquellic <sup>2</sup> , Lovas <sup>1</sup> , Scherschligt <sup>1</sup> , Douglass <sup>1</sup>	mm spectrum assigned
C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> (_CH <sub>2</sub> C(O)CH=CHO_)	3(2H)-furanone 	Lovas <sup>1</sup> , Plusquellic <sup>2</sup> , Suenram <sup>1,5</sup> , Pate <sup>7</sup> , Neill <sup>8</sup> , Muckle <sup>8</sup>	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 <sub>4</sub> H <sub>6</sub> O <sub>3</sub> ( <u>O</u> CHOHC(O)CH <sub>2</sub> C_H <sub>2</sub> )	Dihydro-2-hydroxy- 3(2H)-furanone 	Lovas <sup>1</sup> , Plusquellic <sup>2</sup> , Suenram <sup>1,5</sup> , Pate <sup>7</sup> , Neill <sup>8</sup> , Muckle <sup>8</sup>	Cavity & broadband spectrum assigned, manuscript in prep.
C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> ( <u>O</u> C(O)CHOHCH <sub>2</sub> C_H <sub>2</sub> )	Dihydro-3-hydroxy- 2(3H)-furanone 	Lovas <sup>1</sup> , Plusquellic <sup>2</sup> , Suenram <sup>1,5</sup> , Pate <sup>7</sup> , Neill <sup>8</sup> , Muckle <sup>8</sup>	Cavity & broadband spectrum assigned, manuscript in prep.
C <sub>6</sub> H <sub>15</sub> O <sub>2</sub> N (C <sub>2</sub> H <sub>5</sub> N(CH <sub>2</sub> CH <sub>2</sub> OH) <sub>2</sub> )	<i>N</i> -ethyl diethanol amine	Xu <sup>9</sup> , Liu, <sup>9</sup> Lovas <sup>1</sup> , Suenram <sup>5</sup> , Fraser <sup>1</sup> , Jensen <sup>10</sup> , Samuels <sup>10</sup>	3 Conformers assigned
C <sub>12</sub> H <sub>10</sub> O (C <sub>6</sub> H <sub>5</sub> -O-C <sub>6</sub> H <sub>5</sub> )	Biphenyl ether	Onda <sup>11</sup> , Schnell <sup>12</sup> , Plusquellic <sup>2</sup> , Lovas <sup>1</sup>	Spectrum assigned
H <sub>4</sub> OS (H <sub>2</sub> O-H <sub>2</sub> S)	Hydrogen sulfide - water dimer	Lovas <sup>1</sup> , Suenram <sup>5</sup>	Nine isotopic forms assigned, <b>See Researchgate<sup>a</sup></b>

<sup>a</sup> [https://www.researchgate.net/profile/Francis\\_Lovas/research](https://www.researchgate.net/profile/Francis_Lovas/research)

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>11</sub> H <sub>18</sub> O	Nopol	G. Sedo <sup>1</sup> , F. E. Marshall <sup>2</sup> , G. S. Grubbs II <sup>2</sup>	Manuscript in Preparation
C <sub>10</sub> H <sub>16</sub> O	Myrtenol	G. Sedo <sup>1</sup> , F. E. Marshall <sup>2</sup> , G. S. Grubbs II <sup>2</sup>	<i>J. Mol. Spectrosc.</i> <b>2019</b> , 356, 32-36.
C <sub>10</sub> H <sub>18</sub> O	Endo-(-)-Borneol	G. Sedo <sup>1</sup> , A. J. Duerden <sup>2</sup> , N. Moon <sup>2</sup> , G. Grubbs II <sup>2</sup>	Experiments Completed; 1 conformer assigned

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Formula	Name of Compound	Investigator	Present Stage of Progress
CCl <sup>+</sup>	chloromethyli- dinium	O. Asvany, S. Thorwirth et al.	mmW; ongoing
C <sub>3</sub> HN	cyanoacetylene	L. Bizzocchi, <sup>1</sup> M. Melosso, <sup>2</sup> L. Dore, <sup>2</sup> C. Degli Esposti, <sup>2</sup> F. Tamassia, <sup>3</sup> H. Spahn, <i>et al.</i>	submmW and IR; ongoing; see MPE entry
C <sub>5</sub> H <sub>9</sub> N	2-cyanobutane	K. Borisov, H. S. P. Müller, et al.	search for excited vibrational states; one found
C <sub>3</sub> H <sub>2</sub> O	<i>c</i> -cyclopropenone	A. Brahmi, J.-C. Guillemin, <sup>4</sup> et al.	≤ 505 GHz; various isotopic species. Analysis completed.
C <sub>2</sub> H <sub>6</sub> O (CH <sub>3</sub> ) <sub>2</sub> O	dimethyl ether	C. P. Endres, B. Drouin, <sup>5</sup> V. V. Ilyushin, <sup>6</sup> <i>et al.</i>	$\nu_1 + \nu_2 = 1$ ms. near subm.; higher- $\nu$ ongoing
CO	carbon monoxide	R. Gendriesch, F. Lewen, G. Klapper, H. S. P. Müller	full ms. in prep.
HC <sub>5</sub> N	cyanodiacetylene	T. F. Giesen, J.-U. Grabow, <sup>7</sup> <i>et al.</i>	<i>J. Mol. Spectrosc.</i> , submitted.
C <sub>2</sub> H <sub>5</sub> NO (CH <sub>3</sub> C(O)NH <sub>2</sub> )	acetamide	V. V. Ilyushin <sup>6</sup> <i>et al.</i>	≤ 660 GHz; analysis ongoing
CH <sub>4</sub> S	CH <sub>3</sub> SH, CH <sub>3</sub> <sup>34</sup> SH, <sup>13</sup> CH <sub>3</sub> SH	V. V. Ilyushin, <sup>6</sup> E. Zakharen- ko, L.-H. Xu, <sup>8</sup> R. M. Lees, <sup>8</sup> et al.	≤ 1.5 THz, $\nu_t \leq 2$ ; <sup>34</sup> S species: <i>Astron. Astrophys.</i> <b>627</b> (2019) A41; main species: <b>629</b> (2019) A73; <sup>13</sup> C species: <i>Can. J.</i> <i>Phys.</i> , in press, doi: 10.1139/cjp-2019-0421; main species, higher $\nu$ ongoing.
CH <sub>2</sub> S (H <sub>2</sub> CS)	thioformaldehyde	H. S. P. Müller, A. Maeda, <sup>9</sup> <i>et al.</i>	≤ 1.4 THz; various vib. states; measurements completed
O <sub>2</sub> 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 monofluorides	H. S. P. Müller, S. Thorwirth, <i>et al.</i>	$J'' = 0, 1$ , $\nu \leq 30$ ; preliminary analysis completed

Formula	Name of Compound	Investigator	Present Stage of Progress
C <sub>2</sub> H <sub>3</sub> N (CH <sub>3</sub> CN)	methyl cyanide	H. S. P. Müller, B. J. Drouin, <sup>5</sup> J. C. Pearson, <sup>5</sup> <i>et al.</i>	various vibrational states and isotopic species; ongoing; inclusion of $\nu_4 = 1$ advanced.
O <sub>2</sub> Ti	titanium dioxide	H. S. P. Müller, S. Brünken, <i>et al.</i>	full manuscript on 7 isotopic species in preparation
H <sub>2</sub> N	amidogen	H. S. P. Müller, B. J. Drouin <sup>5</sup>	around 2.6 THz at JPL
C <sub>3</sub> H <sub>6</sub> O (CH <sub>3</sub> C(O)CH <sub>3</sub> )	acetone	M. Ordu <i>et al.</i>	with one <sup>13</sup> C; ≤ 910 GHz; <sup>13</sup> C <sub>2</sub> : <i>Astron. Astrophys.</i> <b>629</b> (2019) A72; measurements of <sup>13</sup> C <sub>1</sub> about to start
CH <sub>6</sub> N <sup>+</sup> (CH <sub>3</sub> NH <sub>3</sub> <sup>+</sup> )	protonated methyl- amine	P. Schmid <i>et al.</i>	rot.; measurements completed; manuscript in preparation
CN <sub>2</sub> O; N <sub>2</sub> ⋯CO	nitrogen carbon monoxide vdW complex	L. A. Surin, I. Tarabukin, <sup>10</sup> S. Schlemmer	"hot band" to doubly excited bending mode; <i>J. Mol. Spec-</i> <i>trosc.</i> 362 (2019) 21
H <sub>3</sub> HeN He⋯NH <sub>3</sub>	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 <sub>3</sub> , He⋯ <i>p</i> NH <sub>3</sub>
H <sub>5</sub> N H <sub>2</sub> ⋯NH <sub>3</sub>	ammonia vdW compl. with hydrogen	I. Tarabukin, <sup>10</sup> L. A. Surin, M. Hermanns, S. Schlemmer	search for rotational transi- tions of <i>p</i> H <sub>2</sub> ⋯ <i>o</i> NH <sub>3</sub> , <i>p</i> H <sub>2</sub> ⋯ <i>p</i> NH <sub>3</sub> and symmetri- cally deuterated isotopologs
H <sub>3</sub> NNe Ne⋯NH <sub>3</sub>	ammonia vdW compl. with neon	I. Tarabukin, <sup>10</sup> L. A. Surin, M. Hermanns, S. Schlemmer	MW; search for rot. trans. of Ne⋯ <i>p</i> NH <sub>3</sub>
H <sub>3</sub> N <sub>3</sub> N <sub>2</sub> ⋯NH <sub>3</sub>	ammonia vdW compl. with nitrogen	I. Tarabukin, <sup>10</sup> L. A. Surin, M. Hermanns, S. Schlemmer	12–28 GHz; completed, ms. in preparation
CN <sup>+</sup>		S. Thorwirth <i>et al.</i>	<i>Astrophys. J. Lett.</i> <b>882</b> (2019) L6.
C <sub>4</sub> H <sub>7</sub> N <i>n</i> -C <sub>3</sub> H <sub>7</sub> CN	<i>n</i> -propyl cyanide	A. Walters, <sup>11</sup> <i>et al.</i>	search for higher vib. states of <i>gauche</i> and <i>anti</i> conformers; ongoing
C <sub>2</sub> H <sub>2</sub> O <sub>3</sub>	formic acid anhydride	A. Walters, <sup>11</sup> J.-C. Guillemin, <sup>4</sup> <i>et al.</i>	measurements and analysis started
C <sub>5</sub> H <sub>9</sub> N	3-methylbutyronitril e	N. Wehres, <i>et al.</i>	≤ 405 GHz; search for excited states ongoing; some found
CH <sub>4</sub> O	CH <sub>3</sub> OD	L.-H. Xu, <sup>8</sup> R. M. Lees, <sup>8</sup> <i>et al.</i>	≤ 1.34 THz, $\nu_t \leq 2$ ; ongoing
CH <sub>4</sub> O	<sup>13</sup> CH <sub>3</sub> OD	L.-H. Xu, <sup>8</sup> R. M. Lees, <sup>8</sup> <i>et al.</i>	≤ 510 GHz, $\nu_t \leq 2$ ; ongoing
C <sub>3</sub> H <sub>6</sub> O	propanal	O. Zingsheim <i>et al.</i>	excited states; further studies ongoing

Formula	Name of Compound	Investigator	Present Stage of Progress
ANALYSIS/ DATABASE	Cologne Database for Molecular Spectroscopy: <a href="http://cdms.astro.uni-koeln.de/">http://cdms.astro.uni-koeln.de/</a>		

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_2H_7N$ $CH_3NHCH_3$	Dimethyl amine	L. Nguyen, <sup>1</sup> C. Gutlé <sup>1</sup> K. Koziol, <sup>2</sup> W. Stahl <sup>2</sup>	Manuscript in Preparation
$C_3H_3D_3O_2$ ( $CD_3COOCH_3$ )	Methyl acetate-D <sub>3</sub> & Methyl-D <sub>3</sub> acetate	L. Nguyen, <sup>1</sup> I. Kleiner <sup>1</sup> L.W. Sutikdja <sup>2,*</sup>	Assignments Completed
$C_3H_9N$ $C_2H_5NHCH_3$	Ethyl methyl amine	L. Nguyen, <sup>1</sup> K. Koziol <sup>2</sup>	Manuscript in Preparation
$n-C_4H_5NS$ $n = 2, 4, 5$	n-Methylthiazol	L. Nguyen, I. Kleiner	$n = 2$ : <i>J. Chem. Phys.</i> 2020 $n = 4, 5$ : Fits in Progress
$C_4H_7NO$ $CH_3(CONH)C_2H_5$	N-Vinylacetamide	L. Nguyen, <sup>1</sup> I. Kleiner <sup>1</sup> R. Kannengießer <sup>2,*</sup>	A Species Assignments Completed, E Species in Progress
$C_4H_8O_2$ $CH_3COOC_2H_5$	Ethyl acetate	L. Nguyen	<i>gauche</i> Conformer: Assignments in Progress
$C_4H_8OS$ $CH_3(C=O)SC_2H_5$	Ethyl thioacetate	L. Nguyen, <sup>1</sup> W. Stahl <sup>2</sup> L. Tulimat <sup>2,*</sup>	Assignments in Progress
$C_4H_{11}N$ ( $CH_3$ ) <sub>3</sub> NH <sub>2</sub>	<i>tert</i> -Butyl amine	L. Nguyen	Assignments Completed, Fits in Progress
$n-C_5H_6N_2$ $n = 2, 4, 5$	n-Methylpyrimidine	T. Nguyen <sup>1</sup> , I. Kleiner <sup>1</sup> , W. Stahl <sup>2</sup>	Assignments Completed, Fits in Progress
$C_5H_4OS$	2-Thiophene- carboxaldehyde	L. Nguyen, <sup>1</sup> H. Mouhib <sup>3</sup> R. Hariki <sup>3,4</sup>	<i>Mol. Phys.</i> 2020 (HRMS2019 issue)
$C_5H_6O_2$ $CH_3C\equiv CCOOCH_3$	Methyl-2-butynoate	L. Nguyen, <sup>1</sup> I. Kleiner <sup>1</sup> K. Eibl <sup>2,*</sup>	Manuscript in Preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
n-C <sub>5</sub> H <sub>7</sub> N n = 1, 2, 3	n-Methylpyrrole	T. Nguyen, I. Kleiner, L. Nguyen	n = 1: Fit in Progress n = 2: <i>Mol. Phys.</i> 2019 (HRMS2019 issue) n = 3: Manuscript in Preparation
C <sub>5</sub> H <sub>7</sub> NS	4,5-Dimethylthiazole	L. Nguyen, <sup>1</sup> T. Nguyen, <sup>1</sup> I. Kleiner, <sup>1</sup> W. Stahl <sup>2</sup> V. Van <sup>2,*</sup>	<i>J. Mol. Struct.</i> 2020 (VSI Hougen)
C <sub>5</sub> H <sub>7</sub> NS	2,4-Dimethylthiazole	S. Khemissi, <sup>1</sup> L. Nguyen, <sup>1</sup> I. Kleiner, <sup>1</sup> V. Van <sup>2</sup>	Assignments in Progress
C <sub>5</sub> H <sub>8</sub> O CH <sub>3</sub> C≡CCH(OH)CH <sub>3</sub>	3-Pentyn-2-ol	L. Nguyen, <sup>1</sup> I. Kleiner <sup>1</sup> K. Eibl <sup>2,*</sup>	Manuscript in Preparation
C <sub>5</sub> H <sub>8</sub> O CH <sub>3</sub> COOCH <sub>2</sub> CH=CH <sub>2</sub>	Allyl acetate	L. Nguyen	Higher Energy Conformers: Assignments in Progress
C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	Coffee furanone	L. Nguyen, <sup>1</sup> W. Stahl, <sup>2</sup> V. Van <sup>2,*</sup>	<i>Can. J. Phys.</i> 2019
C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> N	<i>N</i> -acetyl- <i>N</i> -methylacetamide	K. Eibl, <sup>2,*</sup> R. Kannengießer, <sup>2,*</sup> L. Nguyen <sup>1</sup>	Manuscript in Preparation
C <sub>5</sub> H <sub>11</sub> NO H(CONH)C <sub>4</sub> H <sub>9</sub>	<i>tert</i> -Butylformamide	L. Nguyen, <sup>1</sup> R. Kannengießer <sup>2,*</sup>	Manuscript in Preparation
C <sub>5</sub> H <sub>13</sub> N (CH <sub>3</sub> ) <sub>3</sub> NHCH <sub>3</sub>	<i>N</i> -methyl- <i>tert</i> -butyl amine	L. Nguyen	Assignments Completed, Fits in Progress
C <sub>6</sub> H <sub>7</sub> NS	4-Methyl-5-vinylthiazole	S. Khemissi	Assignment in Progress
C <sub>6</sub> H <sub>8</sub> O	2-Ethylfuran	L. Nguyen	<i>J. Mol. Struct.</i> 2020 (VSI Hougen)
C <sub>5</sub> H <sub>13</sub> N (CH <sub>3</sub> ) <sub>3</sub> NHCH <sub>3</sub>	<i>N</i> -methyl- <i>tert</i> -butyl amine	L. Nguyen <sup>1</sup>	Assignments Completed, Fits in Progress
C <sub>6</sub> H <sub>8</sub> O	2,3-Dimethylfuran	L. Nguyen, <sup>1</sup> I. Kleiner <sup>1</sup> H. Mouhib, <sup>4</sup> R. Hariki <sup>3,4</sup>	Assignment in Progress
C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> CH <sub>3</sub> C≡CCOOCH <sub>2</sub> CH <sub>3</sub>	Ethyl-2-butynoate	L. Nguyen, <sup>1</sup> I. Kleiner <sup>1</sup> K. Eibl <sup>2,*</sup>	2,5: Manuscript in Preparation 2,4: Fits in Progress
C <sub>6</sub> H <sub>9</sub> N	n,m-dimethylpyrrole n,m = 2,4; 2,5	T. Nguyen, I. Kleiner, L. Nguyen	Manuscript in Preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>6</sub> H <sub>9</sub> NS	2,4,5-trimethylthiazole	S. Khemissi	Assignment in Progress
C <sub>6</sub> H <sub>12</sub> O CH <sub>3</sub> COC <sub>4</sub> H <sub>9</sub>	2-Hexanone	M. Andresen <sup>1,2</sup>	<i>ChemPhysChem</i> 2019
C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> COOC <sub>2</sub> H <sub>5</sub>	Ethyl butyrate	L. Nguyen, <sup>1</sup> L.W. Sutikdja <sup>2,*</sup>	Manuscript in Preparation
C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> C <sub>4</sub> H <sub>9</sub> COOCH <sub>3</sub>	<i>n</i> -Methyl pentanoate	L. Nguyen, <sup>1</sup> M. Andresen <sup>1,2</sup>	Manuscript in Preparation
C <sub>6</sub> H <sub>17</sub> NO (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N-H <sub>2</sub> O	Triethyl amine - water	L. Nguyen, <sup>1</sup> R. Kannengießer <sup>2,*</sup>	Assignments in Progress
C <sub>7</sub> H <sub>14</sub> O CH <sub>3</sub> COC <sub>5</sub> H <sub>11</sub>	2-Heptanone	M. Andresen <sup>1,2</sup>	<i>J. Phys. Chem. A</i> 2019
C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> C <sub>5</sub> H <sub>11</sub> COOCH <sub>3</sub>	<i>n</i> -Methyl hexanoate	L. Nguyen <sup>1</sup>	Manuscript in Preparation
C <sub>7</sub> H <sub>10</sub> O <sub>4</sub>	Dimethyl-cyclopropane-1,1-dicarboxylate	L. Nguyen, <sup>1</sup> W. Stahl <sup>2</sup> V. Van, <sup>2,*</sup> P. Groner <sup>5</sup>	Manuscript in Preparation
C <sub>7</sub> H <sub>11</sub> N	1,2,5-Trimethylpyrrole	L. Nguyen, <sup>1</sup> W. Stahl, <sup>2</sup> V. Van <sup>2,*</sup>	Manuscript in Preparation
C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> CH <sub>3</sub> COOC <sub>6</sub> H <sub>5</sub>	Phenyl acetate	L. Nguyen, <sup>1</sup> W. Stahl, <sup>2</sup> L. Ferres <sup>2,*</sup>	Assignments Completed, Fit in Progress
C <sub>8</sub> H <sub>8</sub> OS CH <sub>3</sub> COSC <sub>6</sub> H <sub>5</sub>	Phenylthioacetate	L. Nguyen, <sup>1</sup> W. Stahl, <sup>2</sup> L. Ferres <sup>2,*</sup>	Assignments Completed, Fit in Progress
C <sub>8</sub> H <sub>9</sub> F F(C <sub>6</sub> H <sub>3</sub> )(CH <sub>3</sub> ) <sub>2</sub>	<i>n,m</i> - Dimethylfluorobenzene <i>n,m</i> = 2,3; 2,4; 2,5; 2,6; 3,4; 3,5	S. Khemissi, L. Nguyen	3,5: Assignment in Progress All other isomers: Manuscript in Preparation
C <sub>8</sub> H <sub>12</sub> S	Tetramethylthiophene	L. Nguyen, <sup>1</sup> W. Stahl, <sup>2</sup> V. Van <sup>2,*</sup>	Assignments Completed, Fits in Progress
C <sub>9</sub> H <sub>6</sub> O <sub>2</sub>	Coumarin	L. Nguyen, <sup>1</sup> J.-U. Grabow <sup>6</sup>	Manuscript in Preparation
C <sub>9</sub> H <sub>12</sub> O	<i>n,m</i> -Dimethylanisole <i>n,m</i> = 2,5; 2,6; 3,5	L. Nguyen, <sup>1</sup> W. Stahl, <sup>2</sup> L. Ferres <sup>2,*</sup>	Fits Completed, 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 <sub>4</sub> H <sub>12</sub> [CH <sub>4</sub> C <sub>3</sub> H <sub>8</sub> ]	methane propane	K. I. Peterson <sup>c</sup> , D. P. Pullman <sup>e</sup> , W. Lin, <sup>k</sup> A. J. Minei, <sup>q</sup> E. A. Arsenault, S. E. Novick	J. Phys. Chem. A <b>356</b> , 5274 (2019).
C <sub>3</sub> H <sub>5</sub> F <sub>5</sub> S [CH <sub>3</sub> CH=CH-SF <sub>5</sub> ]	propen-1-ylsulfur pentafluoride	W. Orellana, S. L. Stephens, W. C. Pringle, S. E. Novick, S. A. Cooke <sup>p</sup>	In press, J. Mol. Spectrosc. (2020).
C <sub>4</sub> H <sub>7</sub> F <sub>5</sub> S [CH <sub>3</sub> CH <sub>2</sub> CH=CH-SF <sub>5</sub> ]	buten-1-ylsulfur pentafluoride	W. Orellana, S. L. Stephens, W. C. Pringle, S. E. Novick, S. A. Cooke <sup>p</sup>	In press, J. Mol. Spectrosc. (2020).
C <sub>6</sub> H <sub>5</sub> F <sub>5</sub> S [C <sub>6</sub> H <sub>5</sub> -SF <sub>5</sub> ]	phenylsulfur pentafluoride	J. A. Signore, C. B. Falls, S. L. Stephens, C. A. Jimenez-Hoyos, D. A. Obenchain, <sup>ah</sup> S. A. Cooke, <sup>p</sup> S. E. Novick	J. Mol. Struct. <b>1214</b> , 128130 (2020).
C <sub>3</sub> H <sub>6</sub> NO <sub>3</sub>	n-propyl nitrate	W. Orellana, S. L. Stephens, S. E. Novick, S. A. Cooke, <sup>p</sup> C. Brauer, <sup>d</sup> T. A. Blake <sup>d</sup>	manuscript in preparation
CB <sub>2</sub> F <sub>2</sub>	dibromodifluoromethane	J. A. Signore, C. B. Falls, D. A. Obenchain, <sup>ah</sup> W. C. Pringle, S. A. Cooke, <sup>p</sup> S. E. Novick	manuscript in preparation
C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub>	n-butyl nitrate	S. L. Stephens, J. A. Signore, C. Brauer, <sup>d</sup> T. A. Blake <sup>d</sup> , S. A. Cooke, <sup>p</sup> S. E. Novick	manuscript in preparation
C <sub>7</sub> H <sub>7</sub> I	3-iodotoluene	J. A. Signore, L. Nguyen, <sup>ai</sup> S. A. Cooke, <sup>p</sup> S. E. Novick	work in progress
C <sub>5</sub> H <sub>11</sub> I	1-iodopentane	S. L. Stephens, J. A. Signore, L. Cheng, <sup>af</sup> W. C. Bailey, <sup>ag</sup> S. A. Cooke <sup>p</sup> , S. E. Novick	manuscript in preparation
C <sub>6</sub> H <sub>13</sub> I	1-iodohexane	S. L. Stephens, J. A. Signore, S. A. Cooke, <sup>p</sup> S. E. Novick	work in progress
C <sub>6</sub> H <sub>12</sub>	2-methyl-1-hexen-3-yne	S. L. Stephens, Z. Khanna, R. K. Bohn, S. E. Novick, S. A. Cooke <sup>p</sup>	work in progress
C <sub>6</sub> H <sub>8</sub> O	3-hexyne-2-one	S. L. Stephens, Z. Khanna, R. K. Bohn, S. E. Novick, S. A. Cooke <sup>p</sup>	work in progress



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>3</sub> F <sub>5</sub> O <sub>4</sub> [CF <sub>3</sub> CF <sub>2</sub> COOH HCOOH]	perfluoropropionic acid formic acid	D. A. Obenchain, W. Lin, <sup>k</sup> S. E. Novick, S. A. Cooke <sup>p</sup>	manuscript in preparation
AgCID <sub>2</sub> AgCIDH [D <sub>2</sub> AgCl] [HD AgCl]	hydrogen silver chloride	D. A. Obenchain, G. S. Grubbs II, <sup>x</sup> D. S. Frank, H. M. Pickett, S. E. Novick	all <i>para</i> and <i>ortho</i> isotopologues assigned, manuscript in preparation
C <sub>3</sub> H <sub>2</sub> F <sub>4</sub> O <sub>2</sub> [CF <sub>3</sub> CFHCOOH]	2,3,3,3-tetrafluoropropionic acid	D. A. Obenchain, <sup>ad</sup> J. Wu, <sup>ac</sup> W. Orellana, X. Xu, <sup>ac</sup> S. A. Cooke, <sup>p</sup> S. E. Novick, W. Lin <sup>k</sup>	manuscript in preparation
C <sub>3</sub> H <sub>4</sub> F <sub>4</sub> O <sub>3</sub> [CF <sub>3</sub> CFHCOOH H <sub>2</sub> O]	2,3,3,3-tetrafluoropropionic acid water complex	D. A. Obenchain, <sup>ad</sup> J. Wu, <sup>ac</sup> W. Orellana, X. Xu, <sup>ac</sup> S. A. Cooke, <sup>p</sup> S. E. Novick, W. Lin <sup>k</sup>	manuscript in preparation
C <sub>3</sub> H <sub>7</sub> F <sub>5</sub> O <sub>5</sub> [(H <sub>2</sub> O) <sub>3</sub> CF <sub>3</sub> CF <sub>2</sub> COOH]	pentafluoropropionic acid trihydrate	G. S. Grubbs II, <sup>x</sup> D. A. Obenchain, D. S. Frank, S. E. Novick, S. A. Cooke, <sup>p</sup> A. Serrato III, <sup>k</sup> W. Lin <sup>k</sup>	spectrum assigned
C <sub>6</sub> H <sub>5</sub> F <sub>7</sub> O <sub>2</sub> [CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> COOCH <sub>2</sub> CH <sub>3</sub> ]	ethyl heptafluorobutyrate	B. E. Long, D. S. Frank, L. Hansen, D. Obenchain, R. K Bohn, <sup>r</sup> S. E. Novick	mostly assigned, multiple conformations, work in prog
C <sub>3</sub> H <sub>10</sub> O [H <sub>2</sub> O CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub> ]	water propane ( <sup>13</sup> C isotopomers)	D. A. Obenchain, W. Lin, <sup>k</sup> K. I. Peterson, <sup>e</sup> R. J. Saykally, <sup>z</sup> W. Lin <sup>k</sup>	assigned
C <sub>8</sub> H <sub>11</sub> NO [NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>2</sub> OH]	4-aminophenyl ethanol	C. Bray, C. R. Rivera, E. A. Arsenault, D. A. Obenchain, S. E. Novick, J. L. Knee	assigned
C <sub>6</sub> H <sub>5</sub> F <sub>5</sub> O <sub>2</sub> [CH <sub>2</sub> CHCH <sub>2</sub> OCCF <sub>2</sub> CF <sub>3</sub> ]	allyl perfluoropropionate	D. S. Frank, S. E. Novick, S. A. Cooke, <sup>p</sup> G. S. Grubbs II	assigned
ClCuH <sub>2</sub> [H <sub>2</sub> CuCl]	hydrogen copper chloride	H. M. Pickett, D. A. Obenchain, G. S. Grubbs II, S. E. Novick	4 isotopologues of <i>p</i> -H <sub>2</sub> CuCl and 1 isotopologue of <i>o</i> -H <sub>2</sub> CuCl measured and assigned
C <sub>3</sub> HF <sub>3</sub> 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 <sup>p</sup>	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 <sub>5</sub> H <sub>5</sub> F <sub>5</sub> O <sub>2</sub> [CF <sub>3</sub> CF <sub>2</sub> COOCH <sub>2</sub> CH <sub>3</sub> ]	ethyl pentafluoropropionate	D. A. Obenchain, B. E. Long, B. E. Baker, R. K. Bohn <sup>r</sup> , S. E. Novick, S. A. Cooke <sup>p</sup>	work in progress, assigned
C <sub>5</sub> H <sub>10</sub> O	2-methyl-3-buten-2-ol	B. E. Long, D. A. Obenchain, S. E. Novick, S. A. Cooke <sup>p</sup>	work in progress, assigned
C <sub>5</sub> H <sub>8</sub> Ne [Ne C <sub>5</sub> H <sub>8</sub> ]	neon methylenecyclobutane	A. J. Minei, <sup>q</sup> W. Lin, <sup>k</sup> L. Kang, <sup>i</sup> W. C. Pringle, S. E. Novick	<sup>20</sup> Ne and <sup>22</sup> Ne isotopomers assigned
C <sub>4</sub> H <sub>9</sub> ArN [Ar C <sub>4</sub> H <sub>7</sub> NH <sub>2</sub> ]	argon aminocyclobutane	D. J. Frohman, W. C. Pringle, S. E. Novick	work in progress
C <sub>5</sub> H <sub>7</sub> NNe [Ne C <sub>4</sub> H <sub>7</sub> CN]	neon cyanocyclobutane	D. J. Frohman, W. Ndugire, S. E. Novick, W. C. Pringle	work in progress
C <sub>5</sub> H <sub>7</sub> ArN [Ar C <sub>4</sub> H <sub>7</sub> CN]	argon cyanocyclobutane	D. J. Frohman, D. A. Obenchain, S. E. Novick, W. C. Pringle	work in progress
C <sub>2</sub> F <sub>2</sub> N [F <sub>2</sub> CCN]	1,1-difluoro-2-nitrile-ethynyl radical	L. Kang, <sup>i</sup> S. E. Novick	manuscript in preparation
C <sub>4</sub> H <sub>7</sub> N	3-pyrroline; 2,5-dihydropyrrole	W. Lin, <sup>k</sup> D. J. Frohman, S. E. Novick	work in progress
C <sub>6</sub> H <sub>10</sub> O	3-methylcyclopentanone	A. J. Minei, <sup>q</sup> W. C. Pringle, S. E. Novick	work in progress
C <sub>6</sub> H <sub>10</sub> ArO [Ar C <sub>6</sub> H <sub>10</sub> O]	argon 3-methylcyclopentanone	A. J. Minei, <sup>q</sup> W. C. Pringle, S. E. Novick	work in progress
C <sub>6</sub> H <sub>10</sub>	methylene cyclopentane	A. J. Minei, <sup>q</sup> W. C. Pringle, S. E. Novick	manuscript in preparation
C <sub>6</sub> H <sub>10</sub> Ar [Ar C <sub>6</sub> H <sub>10</sub> ]	argon methylene cyclopentane	A. J. Minei, <sup>q</sup> W. C. Pringle, S. E. Novick	manuscript in preparation
C <sub>6</sub> H <sub>10</sub> Ne [Ne C <sub>6</sub> H <sub>10</sub> ]	neon methylene cyclopentane	A. J. Minei, <sup>q</sup> W. C. Pringle, S. E. Novick	work in progress
C <sub>2</sub> F <sub>6</sub> O <sub>2</sub> [CF <sub>3</sub> OOCF <sub>3</sub> ]	bis[trifluoromethoxy]peroxide	L. Kang, <sup>i</sup> S. E. Novick	spectroscopy completed
C <sub>4</sub> H <sub>8</sub> ArO [Ar C <sub>4</sub> H <sub>8</sub> O]	argon cyclobutanol	W. Lin, <sup>k</sup> G. Lindeke, T.T.E. Mould, W. Ndugire, S. E. Novick, W. C. Pringle	work in progress
C <sub>3</sub> H <sub>6</sub> S	thietane	D. McCamant, J. Schlier, S. E. Novick, W. C. Pringle	manuscript in preparation
C <sub>3</sub> H <sub>6</sub> ArS [Ar C <sub>3</sub> H <sub>6</sub> S]	argon thietane	D. McCamant, J. Schlier, S. E. Novick, W. C. Pringle	manuscript in preparation
C <sub>5</sub> H <sub>8</sub> Ar [Ar C <sub>5</sub> H <sub>8</sub> ]	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 <sub>3</sub> DF <sub>2</sub> [F <sub>2</sub> C-C≡CD]	deuterodifluororopynyl radical	L. Kang, <sup>i</sup> S. E. Novick	work in progress
C <sub>3</sub> H <sub>10</sub> Si [(CH <sub>3</sub> ) <sub>3</sub> SiH]	trimethylsilane	L. Kang, <sup>i</sup> S. E. Novick	spectroscopy completed
C <sub>5</sub> H <sub>10</sub> Si [(CH <sub>3</sub> ) <sub>3</sub> SiC≡CH]	trimethylsilylacetylene	L. Kang, <sup>i</sup> S. E. Novick	spectroscopy completed
C <sub>7</sub> H <sub>10</sub> Si [(CH <sub>3</sub> ) <sub>3</sub> SiC≡C-C≡CH]	trimethylsilyldiacetylene	L. Kang, <sup>i</sup> S. E. Novick	spectroscopy completed
CIDSi [DSiCl]	deuterated chlorosilylene	L. Kang, <sup>i</sup> S. E. Novick	work in progress
C <sub>3</sub> H <sub>10</sub> Ge [(CH <sub>3</sub> ) <sub>3</sub> GeH]	trimethyl germane	W. Lin, <sup>k</sup> L. Kang, <sup>i</sup> S. E. Novick	work in progress
ANALYSIS/DATABASE	Bibliography of Weakly Bound Complexes	<a href="https://wesfiles.wesleyan.edu/home/snovick/SN_webpage/vdw.pdf">https://wesfiles.wesleyan.edu/home/snovick/SN_webpage/vdw.pdf</a>	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>
AgHO(AgOH)	Silver monohydroxide	H. Hashimoto H. Kubota	FTMW spectrum In progress
AgHS(AgSH)	Silver monohydrosulfide	H. Hashimoto H. Kubota	FTMW spectrum In progress
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
ClNi (NiCl)	Nickel monochloride	E. Y. Okabayashi K. Murase	Excited electronic states In progress
ClPd (PdCl)	Palladium monochloride	Y. Kise	mmW spectrum In progress
FPd (PdF)	Palladium monofluoride	Y. Kise	mmW spectrum In progress
OPd (PdO)	Palladium monoxide	T. Kurahara	mmW spectrum In progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
PdS	Palladium monosulfide	S. Kiyose	mmW spectrum In progress
BrH <sub>2</sub> N	Bromoamine	M. Tanaka	mmW spectrum In progress
C <sub>2</sub> FI (ICCF)	Fluoroiodoacetylene <sup>a</sup>	Y. Shimoyama	FTMW spectrum In progress
C <sub>5</sub> FN (FC <sub>5</sub> N)	Fluorocyanodiacetylene	M. Hibi S. Matsumoto	FTMW spectrum In progress

<sup>a</sup> In collaboration with Prof. T. Ogata

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CHF <sub>2</sub>	Difluoromethyl radical	H. Ozeki S. Saito <sup>1</sup>	Analysis completed Manuscripts in preparation
N <sub>2</sub> O	Nitrous oxide	H. Ozeki S. Abe	isotopologues, pressure broadening measurements
O <sub>3</sub>	Ozone	H. Ozeki S. Bailleux <sup>2</sup>	main and isotopologues at 600 GHz
CH <sub>2</sub> (CD <sub>2</sub> )	Methylene-d <sub>2</sub>	H. Ozeki S. Bailleux <sup>2</sup>	THz spectrum assigned manuscript in preparation
H <sub>2</sub> N (NHD)	Amidogen	K. Kobayashi <sup>3</sup> H. Ozeki	THz spectrum manuscript in preparation
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	5-Methyl Hydantoin	H. Ozeki M. Awazu K. Kobayashi <sup>3</sup>	mmW-spectrum in the ground and vibrational excited states assigned manuscript in preparation
INO <sub>2</sub>	Iodine nitrite	H. Watahiki H. Ozeki S. Bailleux <sup>2</sup>	Spectrum assigned.
ClH	Hydrogen Chloride	H. Ozeki	Pressure broadening measurements
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate	H. Ozeki K. Kobayashi <sup>3</sup> S. Kohjiro <sup>4</sup> K. Kikuchi <sup>5</sup>	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 <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S ((CH <sub>3</sub> ) <sub>2</sub> S...CO <sub>2</sub> )	Dimethyl sulfide... carbon dioxide complex	M.M. Serafin	Numerous lines observed; Stark effect experiments in progress.
C <sub>5</sub> H <sub>10</sub> O ((CH <sub>3</sub> ) <sub>2</sub> O...HCCMe)	Dimethyl ether... propyne complex	M.M. Serafin	Numerous lines observed; in progress.
C <sub>3</sub> H <sub>7</sub> F <sub>3</sub> O ((CH <sub>3</sub> ) <sub>2</sub> O...HCF <sub>3</sub> )	Dimethyl ether... fluoroform complex	W. Caminati <sup>a)</sup>	Normal isotopologue assigned; dipole moment measured. Internal motion analysis.
C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> (HCCH...HCF <sub>3</sub> )	Acetylene...fluoroform complex	M.M. Serafin	Normal, H <sup>13</sup> CCH...HCF <sub>3</sub> and DCCD...HCF <sub>3</sub> spectra assigned; internal motion analysis.
C <sub>4</sub> H <sub>12</sub> Si ((C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> SiH <sub>2</sub> )	Diethylsilane	A.L. Steber, D.A. Obenchain, G.A. Guirgis, <sup>b)</sup> J.L. Neill, <sup>c)</sup> M.T. Muckle, <sup>c)</sup> B.H. Pate <sup>c)</sup>	<sup>29</sup> Si, <sup>30</sup> Si and <sup>13</sup> C analysis of <i>anti-anti</i> , <i>anti-gauche</i> and <i>gauche-gauche</i> conformers using CP-FTMW broadband data. Manuscript in preparation.
C <sub>2</sub> HCl <sub>2</sub> FOS (CHCl <sub>2</sub> F...OCS)	Dichlorofluoromethane... carbonyl sulfide complex	A.L. Steber	Normal isotopologue assigned. Cl nuclear quadrupole hyperfine analysis in progress.
C <sub>2</sub> HCIF <sub>2</sub> OS (CHCIF <sub>2</sub> ...OCS)	Chlorodifluoromethane... carbonyl sulfide complex	A.L. Steber, M.D. Foellmer	Tentative assignment made.
C <sub>2</sub> HCIF <sub>2</sub> O <sub>2</sub> (CHCIF <sub>2</sub> ...CO <sub>2</sub> )	Chlorodifluoromethane... carbon dioxide complex	A.L. Steber, M.D. Foellmer, J.L. Neill, <sup>c)</sup> M.T. Muckle, <sup>c)</sup> B.H. Pate <sup>c)</sup>	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 <sub>4</sub> H <sub>12</sub> Ge (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> GeH <sub>2</sub>	Diethylgermane	A.L. Steber, G.A. Guirgis, J.L. Neill, <sup>c)</sup> M.T. Muckle, <sup>c)</sup> B.H. Pate <sup>c)</sup>	<i>Gauche-gauche</i> , <i>anti-gauche</i> and <i>anti-anti</i> conformers assigned using CP-FTMW data. <sup>13</sup> C spectra assigned for <i>gauche-gauche</i> , <i>anti-gauche</i> conformers.
C <sub>7</sub> H <sub>3</sub> F <sub>5</sub> (C <sub>6</sub> F <sub>5</sub> CH <sub>3</sub> )	Pentafluorotoluene	A.A. Elliott, J.M. Sexton, S.A. Cooke, <sup>d)</sup> G.S. Grubbs II <sup>e)</sup>	Substitution structure and dipole moment; internal motion. Manuscript in preparation.
C <sub>6</sub> ClF <sub>5</sub> (C <sub>6</sub> F <sub>5</sub> Cl)	Chloropentafluorobenzene	A.A. Elliott, J.M. Sexton, J.L. Neill, <sup>c)</sup> M.T. Muckle, <sup>c)</sup> B.H. Pate <sup>c)</sup>	Substitution structure and nuclear hyperfine analysis; dipole moment in progress. Manuscript in preparation.
C <sub>4</sub> H <sub>9</sub> Br	2-bromobutane	D.A. Obenchain, Jung-Jin Oh, <sup>f)</sup> Jihyun Kim <sup>f)</sup> Heesu Jang <sup>f)</sup> Soohyun Ka <sup>f)</sup>	Three conformers assigned. <sup>79</sup> Br and <sup>81</sup> Br nuclear quadrupole hyperfine structure. Manuscript in preparation ( <i>J. Mol. Spectrosc.</i> ).
C <sub>4</sub> H <sub>7</sub> Br	2-bromo-1-butene	Jihyun Kim, <sup>f)</sup> Jung-Jin Oh <sup>f)</sup> Heesu Jang <sup>f)</sup>	<sup>79</sup> Br & <sup>81</sup> Br isotopologues assigned.
C <sub>4</sub> H <sub>7</sub> Br	2-bromo-2-butene	Jihyun Kim, <sup>f)</sup> Jung-Jin Oh <sup>f)</sup> Soohyun Ka <sup>f)</sup>	<sup>79</sup> Br, <sup>81</sup> Br assigned; 2 conformers; internal rotation analysis in progress.
C <sub>4</sub> H <sub>7</sub> Br	4-bromo-1-butene	Jung-Jin Oh <sup>f)</sup> Heesu Jang <sup>f)</sup> Soohyun Ka <sup>f)</sup>	<sup>79</sup> Br, <sup>81</sup> Br assigned for <i>ga</i> and <i>gg</i> conformers.
C <sub>8</sub> H <sub>14</sub> O	2-ethylcyclohexanone	Jihyun Kim, <sup>f)</sup> Jung-Jin Oh <sup>f)</sup>	Normal isotopologue assigned.
C <sub>4</sub> H <sub>8</sub> Si (H <sub>2</sub> C=CH) <sub>2</sub> SiH <sub>2</sub>	Divinylsilane	D.A. Obenchain, G.A. Guirgis <sup>b)</sup>	Three conformers assigned; dipole moments measured. Manuscript in preparation.
C <sub>4</sub> H <sub>6</sub> F <sub>2</sub> Si (H <sub>2</sub> C=CH) <sub>2</sub> SiF <sub>2</sub>	Difluorodivynylsilane	D.A. Obenchain, G.A. Guirgis <sup>b)</sup>	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 <sub>3</sub> BrF <sub>2</sub> O (CHBrF <sub>2</sub> ...H <sub>2</sub> O)	Bromodifluoromethane- water complex	A.J. Thomas, D.A. Obenchain, A.L. Steber, <sup>c)</sup> J.L. Neill, <sup>c)</sup> B.H. Pate, <sup>c)</sup> P. Groner <sup>g)</sup>	Assigned <sup>79</sup> Br, <sup>81</sup> Br isotopologues; all transitions doubled by H <sub>2</sub> O internal rotation. Internal rotation analysis in progress.
C <sub>3</sub> H <sub>4</sub> F <sub>2</sub> (CH <sub>2</sub> F <sub>2</sub> ...HCCH)	Difluoromethane... acetylene complex	D.A. Obenchain, D.L. Jurkowski, A.J. Thomas	Normal isotopologue, <sup>13</sup> C <sub>2</sub> H <sub>2</sub> , <sup>13</sup> CH <sub>2</sub> F <sub>2</sub> assigned; Dipole moment measured. Manuscript in preparation.
C <sub>3</sub> H <sub>6</sub> F <sub>2</sub> (CH <sub>2</sub> F <sub>2</sub> ...C <sub>2</sub> H <sub>4</sub> )	Difluoromethane... ethylene complex	D.A. Obenchain	Normal isotopologue assigned; internal motion analysis.
C <sub>3</sub> H <sub>6</sub> ClF (CH <sub>2</sub> ClF...C <sub>2</sub> H <sub>4</sub> )	Chlorofluoromethane... ethylene complex	D.A. Obenchain C.L. Christenholz	<sup>35</sup> Cl, <sup>37</sup> Cl isotopologues assigned; internal motion analysis in progress.
C <sub>2</sub> H <sub>2</sub> ClFO <sub>2</sub> (CH <sub>2</sub> ClF...CO <sub>2</sub> )	Chlorofluoromethane... carbon dioxide complex	D.A. Obenchain, C.L. Christenholz	<sup>35</sup> Cl, <sup>37</sup> Cl isotopologues assigned; internal motion analysis in progress.
C <sub>3</sub> H <sub>4</sub> F <sub>4</sub> (CHF <sub>3</sub> ...C <sub>2</sub> H <sub>3</sub> F)	Trifluoromethane... vinyl fluoride complex	L.F. Elmuti, S.J. Stettner, R.E. Dorris	Normal isotopologue assigned; A, E states fit in progress using XIAM and BELGI.
C <sub>4</sub> H <sub>8</sub> O	1,2-epoxybutane	R.E. Dorris, C.L. Christenholz	Additional measurements 6–16 GHz. <sup>13</sup> C isotopologues identified.
C <sub>8</sub> H <sub>8</sub> (C <sub>6</sub> H <sub>6</sub> ...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 <sub>3</sub> H <sub>3</sub> BrO <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> Br...CO <sub>2</sub> )	Vinyl bromide...carbon dioxide complex	A.M. Anderton	<sup>79</sup> Br and <sup>81</sup> Br isotopologues assigned.
C <sub>2</sub> HF <sub>3</sub> Ne (C <sub>2</sub> HF <sub>3</sub> ...Ne)	Trifluoroethylene...neon complex	A.M. Anderton	<sup>20</sup> Ne and <sup>22</sup> Ne isotopologues assigned; dipole moment.
C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> (ClH <sub>2</sub> CCH <sub>2</sub> Cl)	<i>gauche</i> -1,2-dichloroethane	E.R. Webster A.S. Dikkumbura R.E. Dorris	( <sup>35</sup> Cl <sub>2</sub> ), ( <sup>37</sup> Cl <sub>2</sub> ), ( <sup>35</sup> Cl, <sup>37</sup> Cl) species assigned; structure fit in progress.
C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> Ne (C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> ...Ne)	1,2-difluorobenzene... neon complex	J.M. Kang <sup>h)</sup> M.L. Grant A.G. Akmeemana S.P. Kamari	<sup>20</sup> Ne and <sup>22</sup> Ne isotopologue tentative assignments.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>2</sub> H <sub>4</sub> ClF	1-chloro-2-fluoroethane	A.S Dikkumbura	Normal, <sup>37</sup> Cl, <sup>13</sup> C isotopologues assigned for <i>gauche</i> conformer; structure fit for <i>gauche</i> ; tentative assignment for <i>anti</i> conformer.
C <sub>8</sub> H <sub>5</sub> F (F(C <sub>6</sub> H <sub>4</sub> )C≡CH)	3-fluorophenylacetylene	Heesu Jang <sup>f)</sup> Soohyun Ka <sup>f)</sup> Jung-Jin Oh <sup>f)</sup>	Manuscript in preparation.
C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub>	2,3-dichloropropene	A.S. Dikkumbura	Normal, <sup>37</sup> Cl and <sup>13</sup> C isotopologues assigned for <i>gauche</i> conformer. Normal and <sup>35/37</sup> Cl species for <i>anti</i> conformer; structure fit in progress.
C <sub>3</sub> F <sub>6</sub>	Perfluoropropene	E.N. Pinter A.L. Steber <sup>i)</sup> B. Arenas <sup>i)</sup> M. Schnell <sup>i)</sup>	Normal and <sup>13</sup> C isotopologues assigned 5–18 GHz; dipole moment. 75–110 GHz analysis in progress. Vibrationally excited states obs.
C <sub>3</sub> ArF <sub>6</sub> (C <sub>3</sub> F <sub>6</sub> ...Ar)	Perfluoropropene...Ar complex	R.E. Dorris	Normal isotopologue assigned.
C <sub>3</sub> H <sub>2</sub> F <sub>2</sub> O <sub>2</sub> (C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ...CO <sub>2</sub> )	<i>cis</i> -1,2-difluoroethene...CO <sub>2</sub> complex	W.C. Trendell	Normal isotopologue assigned. Internal motion analysis in progress.
C <sub>4</sub> H <sub>6</sub> F <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>2</sub>	Vinyl fluoride dimer	M.A. Martinez P. Kannangara	T-shaped form observed; normal and <sup>13</sup> C fits; structure. Published <i>J. Mol. Struct.</i> , <b>1211</b> , (2020), 128038.
C <sub>2</sub> H <sub>3</sub> FNe C <sub>2</sub> H <sub>3</sub> F...Ne	Vinyl fluoride...neon dimer	P. Kannangara M.A. Martinez	<sup>20</sup> Ne fit done; consistent with an effective planar structure. Structural analysis in progress.
C <sub>5</sub> H <sub>3</sub> FO <sub>6</sub> (C <sub>2</sub> H <sub>3</sub> F...(CO <sub>2</sub> ) <sub>3</sub> )	Vinyl fluoride...(CO <sub>2</sub> ) <sub>3</sub> tetramer	P. Kannangara	Normal isotopologue assigned; further analysis in progress.
C <sub>6</sub> H <sub>9</sub> F <sub>3</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>3</sub>	Vinyl fluoride trimer	P. Kannangara	Normal isotopologue assigned; further analysis in progress.
C <sub>9</sub> H <sub>12</sub> F <sub>4</sub> O <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>4</sub> ...CO <sub>2</sub>	(Vinyl fluoride) <sub>4</sub> ...CO <sub>2</sub> pentamer	P. Kannangara B.H. Pate <sup>e)</sup> C.T. West <sup>e)</sup>	Spectrum assigned; work to confirm cluster composition in progress.
C <sub>7</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>3</sub> ...CO <sub>2</sub>	(Vinyl fluoride) <sub>3</sub> ...CO <sub>2</sub> tetramer	P. Kannangara	Spectrum assigned; work to confirm cluster composition in progress.

<b><u>FORMULA</u></b>	<b><u>NAME OF COMPOUND</u></b>	<b><u>NAME OF INVESTIGATOR</u></b>	<b><u>PRESENT STAGE OF PROGRESS</u></b>
C <sub>8</sub> H <sub>9</sub> F <sub>3</sub> O <sub>4</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>3</sub> ...(CO <sub>2</sub> ) <sub>2</sub>	(Vinyl fluoride) <sub>3</sub> ...(CO <sub>2</sub> ) <sub>2</sub> pentamer	P. Kannangara	Spectrum assigned; work to confirm cluster composition in progress.
C <sub>5</sub> H <sub>6</sub> F <sub>2</sub> O <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>2</sub> ...CO <sub>2</sub>	(Vinyl fluoride) <sub>2</sub> ...CO <sub>2</sub> trimer	P. Kannangara B.H. Pate <sup>c)</sup> C.T. West <sup>c)</sup>	Spectrum assigned; work to confirm cluster composition in progress.
C <sub>6</sub> H <sub>6</sub> F <sub>2</sub> O <sub>4</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>2</sub> ...(CO <sub>2</sub> ) <sub>2</sub>	(Vinyl fluoride) <sub>2</sub> ...(CO <sub>2</sub> ) <sub>2</sub> tetramer	P. Kannangara B.H. Pate <sup>c)</sup> C.T. West <sup>c)</sup>	Spectrum assigned; work to confirm cluster composition in progress.
C <sub>8</sub> H <sub>12</sub> F <sub>4</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>4</sub>	Vinyl fluoride tetramer	P. Kannangara	Spectrum assigned; tentatively assigned to tetramer. Work to confirm composition ongoing.
C <sub>5</sub> H <sub>6</sub> F <sub>2</sub> NeO <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> F) <sub>2</sub> ...CO <sub>2</sub> ...Ne	(Vinyl fluoride) <sub>2</sub> ...Ne...CO <sub>2</sub> tetramer?	P. Kannangara B.H. Pate <sup>c)</sup> C.T. West <sup>c)</sup>	Two spectra assigned ( <sup>20</sup> Ne/ <sup>22</sup> Ne?); seems consistent with tetramer predictions; further work in progress.
C <sub>4</sub> H <sub>2</sub> F <sub>2</sub> O <sub>4</sub> C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ...(CO <sub>2</sub> ) <sub>2</sub>	1,1-difluoroethylene...(CO <sub>2</sub> ) <sub>2</sub> trimer	T. Ariyaratne	Normal isotopologue assigned; further analysis in progress.
C <sub>5</sub> H <sub>2</sub> F <sub>2</sub> O <sub>6</sub> C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ...(CO <sub>2</sub> ) <sub>3</sub>	1,1-difluoroethylene...(CO <sub>2</sub> ) <sub>3</sub> tetramer	T. Ariyaratne	Normal isotopologue assigned; further analysis in progress.
C <sub>6</sub> H <sub>6</sub> F <sub>6</sub> (C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ) <sub>3</sub>	1,1-difluoroethylene 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 H.L. Fino B.H. Pate <sup>c)</sup> C.T. West <sup>c)</sup>	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>
HDN	amidogen	L. Bizzocchi <sup>3</sup> , M. Melosso <sup>1</sup> , O. Pirali <sup>4</sup> , M.A. Martin-Drumel <sup>4</sup>	ApJS <b>247</b> , 59 (2020)
D <sub>2</sub> N	amidogen	M. Melosso <sup>1</sup> , O. Pirali <sup>4</sup> , M.A. Martin-Drumel <sup>4</sup>	FIR revised + $\nu_2$ band. Analysis ongoing
HD <sup>15</sup> N	amidogen	M. Melosso <sup>1</sup> , L. Bizzocchi <sup>3</sup> , O. Pirali <sup>4</sup> , M.A. Martin-Drumel <sup>4</sup>	FIR spectrum assigned. Submm measurements ongoing
CN	cyano radical	M. Melosso <sup>1</sup> , L. Bizzocchi <sup>3</sup> , O. Pirali <sup>4</sup> , M.A. Martin-Drumel <sup>4</sup>	Submm + FIR spectrum assigned. Analysis completed
C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> (H <sub>2</sub> NCH <sub>2</sub> CN)	aminoacetonitrile	M. Melosso <sup>1</sup> , O. Pirali <sup>4</sup> , M.A. Martin-Drumel <sup>4</sup>	FIR spectrum. Manuscript in preparation
DH <sub>2</sub> N	ammonia-d <sub>1</sub>	M. Melosso <sup>1</sup> , L. Dore <sup>1</sup> , J. Gauss <sup>13</sup> , C. Puzzarini <sup>1</sup>	JMSP, <i>in press</i> (2020)
D <sub>2</sub> HN	ammonia-d <sub>2</sub>	L. Dore <sup>1</sup> , C. Puzzarini <sup>1</sup> , M. Melosso <sup>1</sup> , Z. Kisiel <sup>8</sup>	HFS analysis ongoing
D <sub>3</sub> N	ammonia-d <sub>3</sub>	L. Dore <sup>1</sup> , C. Puzzarini <sup>1</sup> , M. Melosso <sup>1</sup> , Z. Kisiel <sup>8</sup>	HFS analysis ongoing

ArH <sup>+</sup>	argonium	M. Melosso <sup>1</sup> , L. Dore <sup>1</sup> , L. Bizzocchi <sup>3</sup> , D. Prudenzano <sup>3</sup>	Ar broadening + THz measurements. Manuscript in preparation
C <sub>2</sub> D <sub>3</sub> P (CD <sub>3</sub> CP)	perdeuterated- phosphapropine	C. Degli Esposti <sup>1</sup> , M. Melosso <sup>1</sup> , L. Dore <sup>1</sup> , F. Tamassia <sup>2</sup> , L. Bizzocchi <sup>3</sup>	JMSt <b>1203</b> , 127429 (2020)
CH <sub>2</sub> DCI	chloromethane-d <sub>1</sub>	M. Melosso <sup>1</sup> , A. Pietropolli Charmet <sup>5</sup> , F. Tamassia <sup>2</sup>	JQSRT <b>248</b> , 106982 (2020)
C <sub>2</sub> HF <sub>3</sub> (HFCCF <sub>2</sub> )	trifluoroethene	M. Melosso <sup>1</sup> , A. Pietropolli Charmet <sup>5</sup> , F. Tamassia <sup>2</sup>	JQSRT <b>248</b> , 106980 (2020)
C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> (HCCCH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub>	propargylamine dimer	C. Degli Esposti <sup>1</sup> , M. Melosso <sup>1</sup> , L. Spada <sup>1,7</sup> , A. Maris <sup>1</sup>	MW spectrum. Analysis completed
C <sub>3</sub> H <sub>7</sub> NO (HCCCH <sub>2</sub> NH <sub>2</sub> – H <sub>2</sub> O)	propargylamine – water complex	C. Degli Esposti <sup>1</sup> , M. Melosso <sup>1</sup> , L. Spada <sup>1,7</sup> , A. Maris <sup>1</sup>	MW spectrum. Analysis completed
C <sub>3</sub> H <sub>5</sub> N (HCCCH <sub>2</sub> NH <sub>2</sub> )	propargylamine	F. Tamassia <sup>2</sup> , E. Canè <sup>2</sup> , M. Melosso <sup>1</sup>	FIR spectrum. Analysis completed.
C <sub>3</sub> HNO (OCCHCN)	cyanoketene	M. Melosso <sup>1</sup> , L. Dore <sup>1</sup>	Submm-wave spectrum. Analysis completed
C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> (CH <sub>3</sub> NHCN)	<i>N</i> -cyano-methylamine	D. Prudenzano <sup>3</sup> , L. Bizzocchi <sup>3</sup> , M. Melosso <sup>1</sup>	Measurements ongoing
C <sub>3</sub> HN	cianoacetylene	L. Bizzocchi <sup>3</sup> , F. Tamassia <sup>2</sup> , M. Melosso <sup>1</sup> , L. Dore <sup>1</sup>	Higher excited states. Submm-wave and IR ongoing
C <sub>3</sub> DN	<i>d</i> -cianoacetylene	M. Melosso <sup>1</sup> , L. Bizzocchi <sup>3</sup> , F. Tamassia <sup>2</sup>	IR / submm-wave. Manuscript submitted to JQSRT
C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> (CH <sub>2</sub> OH) <sub>2</sub>	ethylene glycol	M. Melosso <sup>1</sup> , L. Dore <sup>1</sup> , B.A. McGuire <sup>14</sup>	JPCA <b>124</b> , 1, 240-246 (2020)

$C_2H_4O$ ( $CH_2CHOH$ )	vinyl alcohol	M. Melosso <sup>1</sup> , L. Dore <sup>1</sup> , B.A. McGuire <sup>14</sup>	ACS Earth Space Chem. <b>3</b> , 7, 1189-1195 (2019)
$C_4H_5N$ ( <i>c</i> -PrCN)	cyclopropyl cyanide	M. Melosso <sup>1</sup> , L. Bizzocchi <sup>3</sup> , A. Steber <sup>6</sup>	FIR + mm-wave spectrum. Analysis ongoing
$C_3H_9N$ ( <i>n</i> - & <i>i</i> -PrNH <sub>2</sub> )	<i>n</i> - & <i>iso</i> -propylamines	M. Melosso <sup>1</sup> , L. Spada <sup>7</sup> , Q. Gou <sup>9</sup>	JPCA <b>124</b> , 7, 1372-1381 (2020)
$C_7H_7N$ (Ph-CH=NH)	phenylmethanimine	A. Melli <sup>7</sup> , L. Spada <sup>7</sup> , J. Grabow <sup>10</sup>	FTMW + mm spectra. Manuscript in preparation
$C_3H_{11}NO$ ( $C_3H_9N-H_2O$ )	<i>n</i> - & <i>iso</i> -propylamine - water complex	C. Puzzarini <sup>1</sup> , Q. Gou <sup>9</sup> , G. Feng <sup>9</sup>	PCCP <b>22</b> , 5024-5032 (2020)
$C_4H_6S_3F_4$ ( $C_2F_4S_2-C_2H_6S$ )	2,2,4,4-tetrafluoro-1,3- dithiethane - dimethylsulfide complex	L. Spada <sup>7</sup> , D. A. Obenchain <sup>10</sup> , M. Juanes <sup>11</sup>	Structure Spectrum assigned
GeS	germanium sulfide	S. Thorwirth <sup>12</sup> , C. Puzzarini <sup>1</sup> , J. Gauss <sup>13</sup> , et al.	Sub-mmwave spectrum
$C_2S$	thioethenylidene	C. Puzzarini <sup>1</sup> , J. Gauss <sup>13</sup> , et al.	Sub-mmwave spectrum manuscript in preparation
HDS	hydrogen sulfide-d1	C. Puzzarini <sup>1</sup> , J. Gauss <sup>13</sup> , et al.	hfs analysis & THz
CO	Carbon monoxide	C. Puzzarini <sup>1</sup> , et al.	Self, N <sub>2</sub> , O <sub>2</sub> , H <sub>2</sub> , He, Ar broadening
$C_2ClF_3$	trifluorochloro-ethylene	C. Puzzarini <sup>1</sup> , L. Spada <sup>7</sup> , N. Tasinato <sup>7</sup> , P. Stoppa <sup>5</sup> , et al.	<sup>35</sup> Cl, <sup>37</sup> 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 <sub>5</sub> H <sub>11</sub> NO	Prolinol	Loru, Sanz, Pérez <sup>1</sup> , Evagelisti <sup>1</sup> , Pate <sup>1</sup> , Cocinero group <sup>2</sup>	Two conf. assigned structure determined Manuscript in prep.
C <sub>5</sub> H <sub>13</sub> NO <sub>2</sub> (C <sub>5</sub> H <sub>11</sub> NO···H <sub>2</sub> O)	Prolinol-H <sub>2</sub> O	Loru, Sanz, Pérez <sup>1</sup> , Evagelisti <sup>1</sup> , Pate <sup>1</sup> , Cocinero group <sup>2</sup>	Four conf. assigned Manuscript in prep.
C <sub>6</sub> H <sub>18</sub> O <sub>3</sub>	Ethanol trimer	Murugachandran, Peña, Sanz, Lamsabhi <sup>3</sup> , Yañez <sup>3</sup>	Four conf. assigned
C <sub>6</sub> H <sub>15</sub> N	Triethylamine	Peña, Sanz, Myllys <sup>4</sup>	Two new conf. assigned
C <sub>6</sub> H <sub>17</sub> NO	Triethylamine-H <sub>2</sub> O	Peña, Sanz Myllys <sup>4</sup>	One conf. assigned
C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>	Methylnitrophenol	Hussain, Burevschi, Sanz, Nguyen <sup>5</sup> , Kleiner <sup>5</sup>	Analysis finished
C <sub>7</sub> H <sub>9</sub> NO <sub>4</sub>	Methylnitrophenol-H <sub>2</sub> O	Hussain, Burevschi, Sanz, Nguyen <sup>5</sup> , Kleiner <sup>5</sup>	Spectrum assigned
C <sub>7</sub> H <sub>10</sub> O <sub>2</sub> (C <sub>7</sub> H <sub>8</sub> O···H <sub>2</sub> O)	P-cresol-H <sub>2</sub> O	Saxena, Hussain, Burevschi, Sanz	Spectrum assigned
C <sub>9</sub> H <sub>2n+14</sub> O <sub>n+1</sub> (C <sub>9</sub> H <sub>14</sub> O--(H <sub>2</sub> O) <sub>n</sub> )	Cyclooctanone-(H <sub>2</sub> O) <sub>n</sub>	Burevschi, Sanz	Several hydrates assigned, manuscript in prep.
C <sub>10</sub> H <sub>6</sub> O <sub>2</sub>	Naphtoquinone	Sanz, Panchagnula, Saxena, Pérez <sup>1</sup> , Evangelisti <sup>1</sup> , Pate <sup>1</sup>	Spectrum assigned structure determined manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{10}H_7NO_2$	Nitronaphthalene	Saxena,Sanz	Spectrum assigned
$C_{10}H_9NO_3$	Nitronaphthalene- $H_2O$	Saxena,Sanz	Spectrum assigned
$C_{10}H_8O_3$ $C_{10}H_{10}O_4$ $C_{10}H_{12}O_6$	Naphtoquinone- $(H_2O)_{1-3}$	Sanz, Saxena, Panchagnula, Pérez <sup>1</sup> , Evangelisti <sup>1</sup> , Pate <sup>1</sup>	Hydrates assigned manuscript in prep.
$C_{10}H_{10}O$ $C_{10}H_{12}O_2$	Azulene- $(H_2O)_{1,2}$	Saxena, Burevschi, Sanz	Hydrates assigned
$C_{10}H_{12}O_2$	Hinokitiol	Medcraft <sup>6</sup> , Murugachandran, Sanz	Several conf. assigned
$C_{10}H_{14}O$	Carvone	Loru et al.	PCCP 2019, 21, 26111-26116
$C_{10}H_{14}O$	Perillaldehyde	Loru et al.	PCCP 2019, 21, 26111-26116
$C_{10}H_{14+2n}O_{n+1}$ $(C_{10}H_{14}O \cdots (H_2O)_{1,2})$	Perillaldehyde- $(H_2O)_{1,2}$	Vigorito, Loru, Sanz	Several conf. assigned
$C_{10}H_{14}O_3$	Hinokitiol- $H_2O$	Medcraft <sup>6</sup> , Murugachandran, Sanz	Several isomers assigned
$C_{10}H_{16}$	Limonene	Loru et al.	PCCP 2019, 21, 26111-26116
$C_{10}H_{2n+16}O_n$ $(C_{10}H_{16}-(H_2O)_n)$	Limonene- $(H_2O)_n$	Murugachandran, Tang, Peña, Loru, Sanz	Several hydrates and isomers assigned
$C_{10}H_{16}$	Alpha-phellandrene	Medcraft <sup>6</sup> , Murugachandran, Sanz	Several conf. assigned
$C_{10}H_{16}O$	Dihydrocarvone	Tang, Loru, Sanz,	Four conf. assigned Manuscript in prep.
$C_{10}H_{16}O_2S$	Limonene- $SO_2$	Medcraft <sup>6</sup> , Murugachandran, Sanz	Several isomers assigned
$C_{10}H_{16+2n}O_{n+1}$ $(C_{10}H_{16}O-(H_2O)_n)$	Fenchone- $(H_2O)_n$	Loru,Burevschi,Sanz, Dréan <sup>7</sup> , Chrayteh <sup>7</sup>	Several hydrates and conf. assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{10}H_{18}O$	Dihydrocarveol	Loru, Jarman, Sanz	Four conf. assigned Manuscript in prep.
$C_{10}H_{18}O$	Geraniol	Sanz group Mohaib <sup>8</sup> , Kleiner <sup>5</sup>	Spectrum observed one conf. assigned
$C_{10}H_{18}O$ ( $C_{10}H_{16} \cdots H_2O$ )	Alpha-phellandrene- $H_2O$	Medcraft <sup>6</sup> , Murugachandran, Sanz	One isomer assigned
$C_{12}H_{22}O$	Cyclododecanone	Burevschi, Sanz	Seven conf. assigned
$C_{12}H_{24}O_2$ $C_{12}H_{26}O_3$	Cyclododecanone- $(H_2O)_{1,2}$	Burevschi, Sanz	Several hydrates assigned
$C_{15}H_{26}O_4$	Romandolide	Burevschi, Sanz	Seven conf. assigned Manuscript in prep.
$C_{16}H_{22}O$ ( $C_{10}H_{16}O \cdots C_6H_6$ )	Fenchone-benzene	Alonso, Burevschi, Sanz	submitted
$C_{16}H_{22}O_2$ ( $C_{10}H_{16}O \cdots C_6H_5OH$ )	Fenchone-phenol	Alonso, Burevschi, Sanz	submitted
$C_{16}H_{30}O$	Muscone	Burevschi, Sanz	Several conf. assigned
$C_{17}H_{32}O_3$	Helvetolide	Burevschi, Sanz	Six conf. assigned
$C_{17}H_{30}O$	Civetone	Burevschi, Loru, Sanz	Two conf. assigned
$C_{20}H_{12}O_4$	Naphtoquinone dimer	Saxena, Sanz Pérez <sup>1</sup> , Evangelisti <sup>1</sup> , Pate <sup>1</sup>	Spectrum assigned
$C_{20}H_{16}$	Azulene dimer	Saxena, Burevschi, Sanz	One conf. assigned
$C_{20}H_{18}O$ $C_{20}H_{20}O_2$ ( $(C_{10}H_8O)_2 \cdots (H_2O)_{1,2}$ )	(Azulene) $_2$ - $(H_2O)_{1,2}$	Saxena, Sanz	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 <sub>3</sub> H <sub>4</sub> N	Ethyl cyanide	Benjamin E. Arenas, Sébastien Gruet, Amanda L. Steber	Experiments Completed: Most Assignments Completed
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	Imidazole	Benjamin E. Arenas, Gayatri Batra, Amanda L. Steber, B.M. Giuliano <sup>1</sup> , L. Bizzocchi <sup>1</sup> , B. J. Harris <sup>5</sup> , B. H. Pate <sup>5</sup>	A&A 629 (2019) A53. Further manuscript in prep.
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	Methyl acetate (75- 110GHz)	Benjamin E. Arenas, Amanda L. Steber	Experiments Completed: Most Assignments Completed
C <sub>3</sub> H <sub>9</sub> NO	Alaninol	Benjamin E. Arenas, Mariyam Fatima	Manuscript submitted.
C <sub>3</sub> H <sub>9</sub> GeI (CH <sub>3</sub> ) <sub>3</sub> GeI	Trimethyl germanium iodide	David Schmitz	Experiments Completed: Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_{16}O_8$ ( $C_3H_6O_3-(H_2O)_n$ n=1-5)	Glycolaldehyde-water complexes	Cristóbal Pérez	ACIE : DOI: 10.1002/anie.201914888 Another manuscript in prep.
$C_3H_{18}O_9$ ( $C_3H_6O_3-(H_2O)_n$ 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	J. Chem. Phys. <b>152</b> (2020) 164303.
$C_5H_{13}NO$	Valinol	Benjamin E. Arenas, Mariyam Fatima	Manuscript submitted.
$C_6H_{15}NO$	Leucinol	Benjamin E. Arenas, Cristóbal Pérez, Mariyam Fatima	Manuscript submitted.
$C_6H_{15}NO$	<i>iso</i> -Leucinol	Benjamin E. Arenas, Mariyam Fatima, Amanda Steber	Manuscript submitted.
$C_7H_8O$	m-Cresol	Sabrina Zinn, Daniel A. Obenchain	Experiments complete; assignments complete
$C_7H_{12}O_2$ ( $C_6H_8O-CH_3OH$ )	Dimethylfuran-methanol	Mariyam Fatima, Cristóbal Pérez, Daniel A. Obenchain	J. Chem. Phys. <b>152</b> (2020) 164303..
$C_8H_8O$	Vinylphenylether	Mariyam Fatima, Cristóbal Pérez	Experiments Completed: Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_8H_8O$	Styrene oxide monomer (2-8 GHz, 75-110 GHz)	Benjamin E. Arenas, Sérgio Domingos, Pascal Stahl <sup>6</sup>	Experiments Completed: Manuscript in prep.
$C_8H_{16}O_2$	Cyclohexane-methanol	Cristóbal Pérez, Mariyam Fatima	Experiments Completed: Manuscript in prep.
$C_{10}H_{15}NO_2$	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	Phys. Chem. Chem. Phys., <b>21</b> (2019) 26569
$C_{10}H_{18}O_2$ ( $C_{10}H_{16}O-H_2O$ )	Thujone-water complexes	Cristóbal Pérez, Zbigniew Kisiel <sup>2</sup>	Experiments Completed: Manuscript in prep.
$C_{10}H_{20}O$	3,7-Dimethyloct-6-en-1- ol (citronellol)	Chris Medcraft, Sérgio Domingos Pablo Pinacho	Experiments Completed: Manuscript in prep.
$C_{11}H_{11}N$ ( $C_6H_6-C_5H_5N$ )	Benzene-pyridine complexes	Mariyam Fatima, Cristóbal Pérez, Barbara M. Giuliano <sup>1</sup>	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, <sup>4</sup> Helen O. Leung <sup>4</sup>	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
$C_{12}H_9NO_3$ $C_{12}H_{11}NO_4$ $C_{12}H_7NO_2-(H_2O)_n$ n=0,1	Naphthalimide monomer + water complex	Sérgio Domingos	Experiments Completed: Manuscript in prep.
$C_{12}H_{10}$	Acenaphthene (75-110GHz)	Sébastien Gruet, Amanda L. Steber	Manuscript accepted (J. Mol. Spec)
$C_{12}H_8O$	Dibenzofuran	Mariyam Fatima, Cristóbal Pérez, Amanda Steber	Experiments Completed: Most Assignments Completed
$C_{12}H_{10}O$	Diphenylether	Chris Medcraft, Sabrina Zinn, Mariyam Fatima, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{12}H_{12}O_3$ $C_{12}H_{14}O_4$ ( $C_{12}H_8O-(H_2O)_n$ n=1-2)	Dibenzofuran-water complexes	Mariyam Fatima, Amanda L. Steber	PCCP 21 (2019) 16032. Further manuscript in prep.
$C_{12}H_{10}O$ $C_{12}H_{12}O_2$ ( $C_{12}H_8-(H_2O)_n$ n=1-2)	Acenaphthylene-water complexes	Amanda L. Steber	Experiments Completed: Manuscript in prep.
$C_{12}H_{14}O_3$ $C_{12}H_{16}O_4$ ( $C_{12}H_{10}O-(H_2O)_n$ n=2-3)	Diphenylether-water higher-order complexes	Mariyam Fatima, Cristóbal Pérez	Experiments Completed: Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{12}H_{22}O_2$	Menthyl acetate	Anna Krin, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{12}H_{26}O_7$ ( $C_{12}H_{24}O_6 \cdot H_2O$ )	18-Crown-6-water complex	Cristóbal Pérez, Juan Carlos Lopez <sup>3</sup>	Experiments Completed: Manuscript in prep.
$C_{13}H_{12}O_2$ ( $C_{12}H_8O \cdot CH_4O$ )	Dibenzofuran-methanol complexes	Mariyam Fatima, Cristóbal Pérez	PCCP 21 (2019) 16032.
$C_{13}H_{11}NO$ $C_{13}H_{13}NO_2$ ( $C_{13}H_9N \cdot (H_2O)_n$ n=1-2)	Phenanthridine-water complexes	Amanda L. Steber, Cristóbal Pérez, Sébastien Gruet, Donatella Loru	Experiments Completed: Most Assignments Completed. Manuscript in preparation.
$C_{13}H_{12}O$ $C_{13}H_{14}O_2$ $C_{13}H_{16}O_3$ ( $C_{13}H_{10} \cdot (H_2O)_n$ n=1-3)	Fluorene-water complexes	Amanda L. Steber, Sébastien Gruet	Assignments complete: Manuscript in prep.
$C_{13}H_{12}O_2$ $C_{13}H_{14}O_3$ $C_{13}H_{16}O_4$ ( $C_{13}H_{10}O \cdot (H_2O)_n$ n=1-3)	Benzophenone-water complexes	Weixing Li, Pablo Pinacho, María Mar Quesada- Moreno	Experiments Completed: Manuscript in prep.
$C_{13}H_{24}O_3$ ( $C_{10}H_{16}O \cdot C_3H_8O_2$ )	Camphor-1,2-propanediol complexes	Cristóbal Pérez, Anna Krin, Mariyam Fatima	Experiments Completed: Most Assignments Completed
$C_{14}H_{12}O$ $C_{14}H_{14}O_2$ ( $C_{14}H_{10} \cdot (H_2O)_n$ n=1-2)	Phenanthrene-water complexes	Amanda L. Steber, Cristóbal Pérez, Donatella Loru	Experiments Completed: Most Assignments Completed. Manuscript in preparation.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{14}H_{25}NO_2$ ( $C_{14}H_{23}NO-H_2O$ )	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.
$C_{14}H_{22}O_2$ ( $C_7H_{14}O-C_7H_8O$ )	Cyclohexane-methanol-benzyl alcohol complex	Cristóbal Pérez, Mariyam Fatima, Pablo Pinacho	Experiments Completed: Manuscript in prep.
$C_{16}H_{16}O_2$ ( $C_8H_8O$ ) <sub>2</sub>	Styrene oxide dimer	Sérgio Domingos Cristobal Perez	Manuscript Submitted
$C_{16}H_{18}O_2$ ( $C_{12}H_8O-C_4H_{10}O$ )	Dibenzofuran- <i>tert</i> -butylalcohol complex	Mariyam Fatima, Cristóbal Pérez	PCCP 21 (2019) 16032.
$C_{16}H_{20}O$ ( $C_{10}H_{14}O-C_6H_6$ )	Carvone-Benzene complex	Weixing Li, María Mar Quesada-Moreno, Pablo Pinacho	Experiments Completed: Most Assignments Completed
$C_{12}H_{30}O_3$ $C_{16}H_{40}O_4$ ( $C_4H_{10}O$ ) <sub>n</sub> 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.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{18}H_{14}O$ ( $C_{18}H_{12}-H_2O$ )	Tetrahellicene-water complexes	Sérgio Domingos	Angew. Chem. 33 (2019) 58
$C_{18}H_{22}O$	4-Methylbenzylidene	Cristóbal Pérez, Anna Krin	Experiments Completed: Manuscript in prep.
$C_{20}H_{26}O$	Diadamantyl ether	Cristóbal Pérez	Manuscript submitted.
$C_{20}H_{34}O_2$ ( $C_{10}H_{16}O-C_{10}H_{18}O$ )	Camphor-fenchol complex	Mariyam Fatima, María Mar Quesada- Moreno, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{20}H_{40}O_2$ ( $C_{10}H_{20}O$ ) <sub>2</sub>	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, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{22}H_{36}O_2$ $C_{20}H_{30}O-C_2H_6O$	Diadamanthyl ether- EtOH complex	María Mar Quesada- Moreno, Pablo Pinacho, Cristóbal Pérez	Manuscript submitted.
$C_{24}H_{40}O_2$ $C_{20}H_{30}O-C_4H_{10}O$	Diadamanthyl ether- <i>tert</i> - butylalcohol complex	María Mar Quesada- Moreno, Pablo Pinacho, Cristóbal Pérez	Manuscript submitted.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>24</sub> H <sub>22</sub> O C <sub>24</sub> H <sub>24</sub> O <sub>2</sub> C <sub>24</sub> H <sub>26</sub> O <sub>3</sub> (C <sub>12</sub> H <sub>10</sub> ) <sub>2</sub> -(H <sub>2</sub> O) <sub>n</sub> n=1-3)	Acenaphthene dimer-water complex	Amanda L. Steber, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
C <sub>13</sub> H <sub>12</sub> O <sub>2</sub> C <sub>13</sub> H <sub>14</sub> O <sub>3</sub> C <sub>13</sub> H <sub>16</sub> O <sub>4</sub> (C <sub>13</sub> H <sub>10</sub> O-(H <sub>2</sub> O) <sub>n</sub> n=1-3)	Benzophenone-water complexes	Weixing Li, Pablo Pinacho, María Mar Quesada-Moreno	Experiments Completed: Manuscript in prep.
C <sub>16</sub> H <sub>20</sub> O (C <sub>10</sub> H <sub>14</sub> O-C <sub>6</sub> H <sub>6</sub> )	Carvone-benzene complexes	Weixing Li, María Mar Quesada-Moreno, Pablo Pinacho	Experiments Completed: Most Assignments Completed
C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> C <sub>7</sub> H <sub>10</sub> O <sub>3</sub> C <sub>7</sub> H <sub>12</sub> O <sub>4</sub> C <sub>7</sub> H <sub>14</sub> O <sub>5</sub> C <sub>7</sub> H <sub>16</sub> O <sub>6</sub> C <sub>7</sub> H <sub>18</sub> O <sub>7</sub> (C <sub>7</sub> H <sub>6</sub> O-(H <sub>2</sub> O) <sub>n</sub> n=1-6)	benzaldehyde-water complexes	Weixing Li, Amanda L. Steber, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
C <sub>7</sub> F <sub>3</sub> H <sub>3</sub> O <sub>2</sub> C <sub>7</sub> F <sub>5</sub> H <sub>5</sub> O <sub>3</sub> C <sub>7</sub> F <sub>7</sub> H <sub>7</sub> O <sub>4</sub> C <sub>7</sub> F <sub>9</sub> H <sub>9</sub> O <sub>5</sub> C <sub>7</sub> F <sub>5</sub> H <sub>11</sub> O <sub>6</sub> (C <sub>7</sub> HF <sub>5</sub> O-(H <sub>2</sub> O) <sub>n</sub> n=1-5)	Pentafluorobenzaldehyde-water complexes	Weixing Li, Cristóbal Pérez, Amanda L. Steber	Experiments Completed: Manuscript in prep.
C <sub>7</sub> H <sub>7</sub> FO <sub>2</sub> C <sub>7</sub> H <sub>9</sub> FO <sub>3</sub> C <sub>7</sub> H <sub>11</sub> FO <sub>4</sub> (C <sub>7</sub> H <sub>5</sub> FO-(H <sub>2</sub> O) <sub>n</sub> n=1-3)	2-Fluorobenzaldehyde-water complexes	Weixing Li	Experiments Completed: Most Assignments Completed
C <sub>7</sub> H <sub>7</sub> FO <sub>2</sub> C <sub>7</sub> H <sub>9</sub> FO <sub>3</sub> C <sub>7</sub> H <sub>11</sub> FO <sub>4</sub> (C <sub>7</sub> H <sub>5</sub> FO-(H <sub>2</sub> O) <sub>n</sub> n=1-3)	3-Fluorobenzaldehyde-water complexes	Weixing Li	Experiments Completed: Most Assignments Completed
C <sub>7</sub> H <sub>7</sub> FO <sub>2</sub> C <sub>7</sub> H <sub>9</sub> FO <sub>3</sub> C <sub>7</sub> H <sub>11</sub> FO <sub>4</sub> (C <sub>7</sub> H <sub>5</sub> FO-(H <sub>2</sub> O) <sub>n</sub> n=1-3)	4-Fluorobenzaldehyde-water complexes	Weixing Li	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 <sub>8</sub> H <sub>7</sub> FO <sub>3</sub> C <sub>9</sub> H <sub>9</sub> FO <sub>5</sub> (C <sub>7</sub> H <sub>5</sub> FO-(CH <sub>2</sub> O <sub>2</sub> ) <sub>n</sub> n=1-2)	2-Fluorobenzaldehyde-formic acid complexes	Weixing Li	Experiments Completed: Manuscript in prep.
C <sub>7</sub> H <sub>7</sub> FO <sub>2</sub> C <sub>8</sub> H <sub>9</sub> FO <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> F-(CH <sub>2</sub> O <sub>2</sub> ) <sub>n</sub> n=1-2)	Fluorobenzene-formic acid complexes	Weixing Li	Experiments Completed: Manuscript in prep.
C <sub>14</sub> H <sub>12</sub> O <sub>2</sub> (C <sub>10</sub> H <sub>8</sub> O-(C <sub>4</sub> H <sub>4</sub> O))	2-naphthol - furan complex	Daniel A. Obenchain, María Mar Quesada-Moreno	Experiments Completed: Manuscript in prep.
C <sub>16</sub> H <sub>16</sub> O <sub>2</sub> (C <sub>10</sub> H <sub>8</sub> O-(C <sub>6</sub> H <sub>8</sub> O))	2-naphthol - dimethylfuran complex	Daniel A. Obenchain, María Mar Quesada-Moreno	Experiments Completed: Manuscript in prep.
C <sub>14</sub> H <sub>12</sub> OS (C <sub>10</sub> H <sub>8</sub> O-(C <sub>4</sub> H <sub>4</sub> S))	2-naphthol - thiophene complex	Daniel A. Obenchain, María Mar Quesada-Moreno	Experiments Completed: Manuscript in prep.
C <sub>11</sub> H <sub>8</sub> O <sub>2</sub> (C <sub>10</sub> H <sub>8</sub> O-(CO))	2-naphthol - CO complex	Daniel A. Obenchain, María Mar Quesada-Moreno	Experiments Completed: Manuscript in prep.
C <sub>16</sub> H <sub>14</sub> O (C <sub>10</sub> H <sub>8</sub> O-(C <sub>6</sub> H <sub>6</sub> ))	2-naphthol - benzene complex	Daniel A. Obenchain, María Mar Quesada-Moreno Rizalina Tama Saragi <sup>3</sup>	Experiments Completed: Most Assignments Completed
C <sub>12</sub> H <sub>12</sub> O (C <sub>10</sub> H <sub>8</sub> O-(C <sub>2</sub> H <sub>2</sub> ))	2-naphthol – acetylene complex	Daniel A. Obenchain, María Mar Quesada-Moreno	Assignments Completed Manuscript in prep.
C <sub>12</sub> H <sub>14</sub> O (C <sub>10</sub> H <sub>8</sub> O-(C <sub>2</sub> H <sub>4</sub> ))	2-naphthol – ethylene complex	Daniel A. Obenchain, María Mar Quesada-Moreno	Assignments Completed Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{26}H_{36}O$ ( $C_{20}H_{30}O-(C_6H_6)$ )	Diadamanthyl ether-benzene complex	María Mar Quesada-Moreno, Pablo Pinacho, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{26}H_{35}FO$ ( $C_{20}H_{30}O-(C_6H_5F)$ )	Diadamanthyl ether-monofluorobenzene complex	María Mar Quesada-Moreno, Pablo Pinacho, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_{26}H_{30}F_6O$ ( $C_{20}H_{30}O-(C_6F_6)$ )	Diadamanthyl ether-hexafluorobenzene complexes	María Mar Quesada-Moreno, Pablo Pinacho, Cristóbal Pérez	Experiments Completed: Manuscript in prep.
$C_9H_8$	3-methylphenylacetylene	Daniel A. Obenchain, Pablo Pinacho, Sabrina Zinn	J. Mol. Struct. 1213 (2020) 128109
$C_4H_6O$ ( $C_4H_4O-(H_2)$ )	Furan – hydrogen complex	Daniel A. Obenchain, Pablo Pinacho	Experiments Completed: Most Assignments Completed
$C_6H_{12}O_2$	Cyclohexylhydroperoxide	Pablo Pinacho, Sabrina Zinn	Experiments Completed: Manuscript in prep.
$C_6H_{10}O_4$	Adipic acid	Pablo Pinacho, Sabrina Zinn	Experiments Completed: Manuscript in prep.
$C_6H_{12}O_3$	6-hydroxyhexanoic acid	Pablo Pinacho, Sabrina Zinn	Experiments Completed: Manuscript in prep.
$C_{14}H_{28}O_2$ ( $C_7H_{14}O$ ) <sub>2</sub>	Cyclohexane-methanol dimer	Cristóbal Pérez, Mariyam Fatima, Pablo Pinacho	Experiments Completed: Manuscript in prep.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{14}H_{16}O_2$ ( $C_7H_8O$ ) <sub>2</sub>	Benzyl alcohol dimer	Cristóbal Pérez, Mariyam Fatima, Pablo Pinacho	Experiments Completed: Manuscript in prep.
$C_{20}H_{34}O_2$ ( $C_{10}H_{16}O$ - $C_{10}H_{18}O$ )	Fenchone-fenchol complexes	Daniel A. Obenchain, Pablo Pinacho	Experiments Completed: Manuscript in prep.
$C_9H_{10}O_3$	$\alpha$ -Methoxyphenylacetic acid	Pablo Pinacho, María Mar Quesada- Moreno, Himanshi Singh	Experiments Completed: Manuscript in prep.
$C_{11}H_{16}O_4S$ ( $C_9H_{10}O_3$ - $C_2H_6OS$ )	$\alpha$ -Methoxyphenylacetic acid – DMSO complex	Pablo Pinacho, María Mar Quesada- Moreno, Himanshi Singh	Experiments Completed: Manuscript in prep.
$C_{10}H_{18}O$	Borneol	Pablo Pinacho, María Mar Quesada- Moreno,	Experiments Completed: Manuscript in prep.
$C_{10}H_{18}O$	Isoborneol	Pablo Pinacho, María Mar Quesada- Moreno,	Experiments Completed: Manuscript in prep.
$C_{20}H_{36}O_2$ ( $C_{10}H_{18}O$ ) <sub>2</sub>	Borneol dimer	Pablo Pinacho, María Mar Quesada- Moreno,	Experiments Completed: Manuscript in prep.
$C_{20}H_{36}O_2$ ( $C_{10}H_{18}O$ ) <sub>2</sub>	Isoborneol dimer	Pablo Pinacho, María Mar Quesada- Moreno,	Experiments Completed: Manuscript in prep.
$C_{12}H_{24}O_2S$ ( $C_{10}H_{18}O$ - $C_2H_6OS$ )	Borneol – DMSO complex	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>
$C_{12}H_{24}O_2S$ ( $C_{10}H_{18}O-C_2H_6OS$ )	Isoborneol – DMSO complex	Pablo Pinacho, María Mar Quesada- Moreno	Experiments Completed: Manuscript in prep.
$C_{10}H_{20}O_2$ ( $C_{10}H_{18}O-H_2O$ )	Borneol – water complex	Pablo Pinacho, María Mar Quesada- Moreno	Experiments Completed: Manuscript in prep.
$C_{10}H_{20}O_2$ ( $C_{10}H_{18}O-H_2O$ )	Isoborneol – water complex	Pablo Pinacho, María Mar Quesada- Moreno	Experiments Completed: Manuscript in prep.
$H_8S_3O$ $H_{12}S_3O_3$ $((H_2O)_n-(H_2S)_m)$ [n=1, m=3] & [n=3, m=3]	$H_2S$ – water higher order complexes	Cristóbal Pérez, Pablo Pinacho, Rizalina Tama Saragi <sup>3</sup>	Experiments Completed: Most Assignments Completed
$C_5H_{12}O_2$ ( $C_4H_8O-CH_4O$ )	Tetrahydrofuran – methanol complex	Pablo Pinacho, Rizalina Tama Saragi <sup>3</sup>	Experiments Completed: Most Assignments Completed
$C_6H_{14}O_2$ ( $C_4H_8O-C_2H_6O$ )	Tetrahydrofuran – ethanol complex	Pablo Pinacho, Rizalina Tama Saragi <sup>3</sup>	Experiments Completed: Most Assignments Completed
$C_6H_{11}F_3O_2$ ( $C_4H_8O-C_2H_3F_3O$ )	Tetrahydrofuran – trifluoroethanol complex	Pablo Pinacho, Rizalina Tama Saragi <sup>3</sup>	Experiments Completed: Most Assignments Completed
$C_8H_{18}O_2$ ( $C_4H_8O-C_4H_{10}O$ )	Tetrahydrofuran – <i>tert</i> -butylalcohol complex	Pablo Pinacho, Rizalina Tama Saragi <sup>3</sup>	Experiments Completed: Most Assignments Completed
$C_{10}H_{20}O_2$ ( $C_4H_8O-C_6H_{12}O$ )	Tetrahydrofuran – cyclohexanol complex	Pablo Pinacho, Rizalina Tama Saragi <sup>3</sup>	Experiments Completed: Most Assignments Completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_{13}H_{10}O$	Xanthene	Donatella Loru	Experiments Completed: Most Assignments Completed
$C_{12}H_{10}O$	Acenaphthenol	Donatella Loru, Amanda Steber, Daniel Rap <sup>7</sup>	Experiments Completed: Manuscript in prep.
$C_{24}H_{20}O_2$ (( $C_{12}H_{10}O$ ) <sub>2</sub> )	acenaphthenol dimer	Donatella Loru, Amanda Steber, Daniel Rap <sup>7</sup>	Experiments Completed: Manuscript in prep.
$C_{12}H_{10}O_2$ $C_{12}H_{12}O_3$ $C_{12}H_{14}O_4$ ( $C_{12}H_8O-(H_2O)_n$ n=1-3)	acenaphthenol-water complexes	Donatella Loru, Amanda Steber, Daniel Rap <sup>7</sup>	Experiments Completed: Manuscript in prep.
$C_{12}H_{12}$ $C_{12}H_{14}$ ( $C_{12}H_{10}-(H_2)_n$ n=1,2)	Acenaphthene-hydrogen complexes	Amanda Steber	Experiments completed, Most assignments completed
$C_{13}H_{12}$	Fluorene-hydrogen complexes	Amanda Steber	Experiments completed, Most assignments completed
$C_9H_6N_4$	3,3-dimethyl-tetracyanocyclopropane	Sérgio Domingos Tiddo Mooibroek <sup>8</sup>	Manuscript submitted
$C_{13}H_{14}N_4O$	3,3-dimethyl-tetracyanocyclopropane - tetrahydrofuran	Sérgio Domingos Tiddo Mooibroek <sup>8</sup>	Manuscript submitted
$C_{10}H_{14}O_2$	6-Amyl- $\alpha$ -pyrone	Himanshi Singh, Mariyam Fatima, Cristobal Perez	Experiments completed. Some assignments completed

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>10</sub> H <sub>14</sub> O C <sub>10</sub> H <sub>16</sub> O <sub>2</sub> C <sub>10</sub> H <sub>18</sub> O <sub>3</sub> (C <sub>10</sub> H <sub>14</sub> O-H <sub>2</sub> O)	(S)-5-Allyl-2-oxabicyclo[3.3.0]oct-8-ene monomer and water complexes	Wenhao Sun	Multiple conformers assigned
C <sub>12</sub> H <sub>15</sub> NO <sub>3</sub>	N-alpha-Acetyl-L-phenylalanine methyl ester	Daniel A. Obenchain	Assignments complete, internal rotational analysis
C <sub>14</sub> H <sub>13</sub> BrO (C <sub>8</sub> H <sub>8</sub> O-C <sub>6</sub> H <sub>5</sub> Br)	Styrene oxide – bromobenzene complexes	Daniel A. Obenchain Cristobal Perez	Assignments complete Manuscript in prep.
C <sub>14</sub> H <sub>13</sub> IO (C <sub>8</sub> H <sub>8</sub> O-C <sub>6</sub> H <sub>5</sub> I)	Styrene oxide – iodobenzene complexes	Daniel A. Obenchain Cristobal Perez	Assignments and NQCC analyses ongoing

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FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR	PRESENT STAGE OF PROGRESS
$C_3H_7ClO$ ( $ClCH_2CH_2OCH_3$ )	2-chloroethyl methyl ether	Riffe, Shipman	Refining fits of excited vibrational states.
$C_4H_8O$ ( $CH_2(O)CHCH_2CH_3$ )	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>
$C_4H_{10}S$ $CH_3SC_3H_7$	Methyl propyl sulfide	L. Tulimat*	Manuscript in Preparation
$C_5H_5ClS$	2-Chloro-3-Methylthiophene	K. Koziol	Assignments in Progress
$C_5H_8O$ $CH_3COCH=CHCH_3$	3-Penten-2-one	M. Andresen <sup>1,2</sup>	Manuscript in Preparation
$C_5H_8O$ $CH_3COC(CH_3)=CH_2$	3-Methyl-3-Buten-2-one	M. Andresen <sup>1,2</sup>	Manuscript in Preparation
$C_5H_{10}O$ $CH_3COCH(CH_3)_2$	3-Methyl-2-butanone	M. Andresen <sup>1,2</sup>	Assignment in Progress
$C_6H_6O_2$	2-Acetylfuran	C. Dindic	Assignment in Progress
$C_6H_6OS$	3-Methyl-2-thiophenecarboxaldehyde	C. Dindic	Assignment in Progress
$C_6H_6OS$	2-Acetylthiophene	C. Dindic	Manuscript in Preparation
$C_6H_{10}O$ $CH_3COC_4H_7$	4-Methylpent-3-en-2-one	H. Mouhib <sup>3</sup>	Assignment of Two Rotor Completed, 3 <sup>rd</sup> rotor in Progress
$C_6H_{13}OS$ $CH_3O(CH_2)_2C_3H_6SH$	4-Methoxy-2-methylbutane-2-thiol	H. Mouhib <sup>3</sup>	Manuscript in Preparation
$C_7H_8OS$	2-Propionylthiophene	C. Dindic	Manuscript in Preparation
$C_7H_8OS$	2-Acetyl-3-methylthiophene	C. Dindic	Assignment in Progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>7</sub> H <sub>8</sub> OS	2-Acetyl-4-methylthiophene	C. Dindic	Assignment in Progress
C <sub>8</sub> H <sub>10</sub> OS	3-Acetyl-2,5-dimethylthiophene	C. Dindic	Assignment in Progress
C <sub>8</sub> H <sub>16</sub> O CH <sub>2</sub> =CHCH(OH)C <sub>5</sub> H <sub>11</sub>	Octen-3-ol	H. Mouhib <sup>3</sup>	Manuscript in Preparation
C <sub>9</sub> H <sub>12</sub> O (CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> OCH <sub>3</sub>	2,4-Dimethylansiole	L. Ferres <sup>*</sup>	<i>J. Chem. Phys.</i> 2019
C <sub>10</sub> H <sub>12</sub> O	Rose oxide	H. Mouhib <sup>3</sup> V. Van <sup>1,*</sup>	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 <sub>6</sub> H <sub>7</sub> NO	2-aminophenol	K. Byerly G. A. Laubacher <sup>1</sup> M. J. Tubergen	Spectrum recorded; assignment in progress
C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	guaiacol	A. Fox M. J. Tubergen R. M. Gurusinghe <sup>2</sup>	Spectrum and <sup>13</sup> C isotopomers assigned, argon spectrum assigned; water complex spectra recorded; manuscript in prep.
C <sub>3</sub> H <sub>9</sub> NO	2-methoxyethylamine	N. Harper <sup>3</sup> B. Basenback <sup>4</sup> R. M. Gurusinghe <sup>2</sup> M. J. Tubergen	<sup>13</sup> C isotopomers assigned. Water complex spectrum assigned. manuscript in preparation
C <sub>3</sub> H <sub>11</sub> NO <sub>2</sub>	N-methyl-2-aminoethanol-water	D. Valente <sup>5</sup> D. Marasinghe M. J. Tubergen	spectrum and eQq assigned.
C <sub>9</sub> H <sub>10</sub>	$\alpha$ -Methylstyrene, cis- $\beta$ -Methylstyrene Trans- $\beta$ -Methylstyrene	R. M. Gurusinghe <sup>2</sup> M. J. Tubergen	Spectra assigned including internal Rotation. Manuscript in Preparation
C <sub>3</sub> H <sub>6</sub> ArO <sub>2</sub>	glycidol-argon	R. Wooten-Moyer <sup>6</sup> 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 <sub>7</sub> H <sub>4</sub> NO	phenyl isocyanate	W. Sun, W. Silva	JPC A <b>123</b> (2019) 2351.
C <sub>7</sub> H <sub>5</sub> NS	phenyl isothiocyanate	W. Sun, W. Silva	JPC A <b>123</b> (2019) 2351.
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S	3-mercaptopropionic acid	W. Silva	J. Mol. Spec. <b>362</b> (2019) 1.
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S	methyl 3-mercaptopropionate	W. Silva	JPC A <b>123</b> (2019) 9840.
C <sub>4</sub> H <sub>5</sub> NO	allyl isocyanate	O. Sogeke, W. Sun, W. Silva	JCP <b>151</b> (2019) 194304.
C <sub>7</sub> H <sub>7</sub> FO	2-fluoroanisole	K. Bergmann	JPC A 124 (2020) 2270.
C <sub>7</sub> H <sub>7</sub> FO	3-fluoroanisole	K. Bergmann	JPC A 124 (2020) 2270.
C <sub>8</sub> H <sub>7</sub> F	2-fluorostyrene	S. Stephens	str. analysis in progress
C <sub>8</sub> H <sub>7</sub> F	4-fluorostyrene	S. Stephens	str. analysis in progress
C <sub>3</sub> H <sub>6</sub> S (thietane)	trimethylene sulfide	D. Desmond	MW parent, 13C, 34S, 33S- assigned far IR in progress
C <sub>3</sub> H <sub>6</sub> O (oxetane)	trimethylene oxide	D. Desmond O. Mahassneh	MW parent assigned 13C, 18O done far IR paper in preparation
C <sub>4</sub> H <sub>5</sub> NS	allyl isothiocyanate	J. Stitsky	manuscript submitted
C <sub>8</sub> H <sub>7</sub> NO	benzyl isocyanate	J. Stitsky	str. analysis in progress
C <sub>8</sub> H <sub>7</sub> NS	benzyl isothiocyanate	J. Stitsky	str. analysis in progress



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	trimethylene oxide-water	W. Silva	manuscript in preparation
C <sub>3</sub> H <sub>8</sub> OS	trimethylene sulfide-water	W. Silva	manuscript in preparation
C <sub>4</sub> H <sub>6</sub> OS	thiophene-water	W. Silva	MW spectrum, tunneling
C <sub>6</sub> H <sub>6</sub> FN	2-fluoroaniline	T. Poonia	manuscript in preparation
C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>	3-furaldehyde	C. Gregory	manuscript in preparation
C <sub>6</sub> H <sub>9</sub> N	<i>N</i> -allylmethylamine	W. Silva, T. Poonia	Calculations done, cp-FTMW in progress.
C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	tetrahydrofurfuryl alcohol	W. Silva	Calculations done, cp-FTMW in progress.
C <sub>5</sub> H <sub>11</sub> NO	tetrahydrofurfuryl amine	W. Silva	Calculations done, cp-FTMW in progress.

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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 <sub>3</sub> F <sub>3</sub> IP*	H <sub>3</sub> P...ICF <sub>3</sub>	S. L. Stephens	Spectrum assigned.
CH <sub>3</sub> NS <sub>2</sub> *	H <sub>3</sub> N...CS <sub>2</sub>	E. Gougoula, C. Medcraft	J. Chem. Phys. <b>150</b> , 084307 (2019)
CH <sub>4</sub> ArN <sub>2</sub> O*	CH <sub>4</sub> N <sub>2</sub> O...Ar (urea-argon complex)	C. Medcraft	Spectrum assigned.
CH <sub>4</sub> NOP	OCNH <sub>2</sub> PH <sub>2</sub> (phosphine carboxamide)	E. Gougoula	Spectra of isotopologues assigned Manuscript in preparation
CH <sub>4</sub> ArNOP	OCNH <sub>2</sub> PH <sub>2</sub> ...Ar (phosphine carboxamide-argon complex)	E. Gougoula	Manuscript in preparation
CH <sub>4</sub> ArN <sub>2</sub> S*	CH <sub>4</sub> N <sub>2</sub> S...Ar (thiourea-argon complex)	C. Medcraft	Spectrum assigned.
CH <sub>6</sub> N <sub>2</sub> OS*	CH <sub>4</sub> N <sub>2</sub> S...H <sub>2</sub> O (thiourea-water complex)	C. Medcraft	Spectrum assigned.
C <sub>2</sub> H <sub>2</sub> AgI*	C <sub>2</sub> H <sub>2</sub> ...Ag-I	S. L. Stephens	Spectrum assigned.
C <sub>2</sub> H <sub>2</sub> CuF*	C <sub>2</sub> H <sub>2</sub> ...Cu-F	S.L. Stephens, D.P. Zaleski	Spectrum assigned, isotopic work.
C <sub>2</sub> H <sub>2</sub> CuI*	C <sub>2</sub> H <sub>2</sub> ...Cu-I	S. L. Stephens, D. Bittner	Spectrum assigned.
C <sub>2</sub> H <sub>4</sub> AgF*	C <sub>2</sub> H <sub>4</sub> ...Ag-F	S. L. Stephens	Spectrum assigned.
C <sub>2</sub> H <sub>4</sub> AgI*	C <sub>2</sub> H <sub>4</sub> ...Ag-I	S. L. Stephens	Spectrum assigned.
C <sub>2</sub> H <sub>4</sub> AuI*	C <sub>2</sub> H <sub>4</sub> ...Au-I	S. L. Stephens, M. Sprawling, D. P. Zaleski	Spectra of isotopologues assigned, manuscript in preparation.
C <sub>2</sub> H <sub>4</sub> CuF*	C <sub>2</sub> H <sub>4</sub> ...Cu-F	S. L. Stephens	Spectrum assigned.
C <sub>2</sub> H <sub>4</sub> CuI*	C <sub>2</sub> H <sub>4</sub> ...Cu-I	S. L. Stephens	Spectrum assigned.
C <sub>3</sub> H <sub>2</sub> F <sub>3</sub> I*	C <sub>2</sub> H <sub>2</sub> ...ICF <sub>3</sub>	S. L. Stephens	Manuscript in preparation
C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub>	4(5)-nitroimidazole	E. Gougoula	Spectrum assigned
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ...H <sub>2</sub> O	E. Gougoula, D. J. Cole	J. Phys. Chem A, DOI: 10.1021/acs.jpca.0c00544

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>3</sub> H <sub>9</sub> AgNI*	(CH <sub>3</sub> ) <sub>3</sub> N...Ag-I	D. Bittner, S. L. Stephens	Spectrum assigned. Manuscript in preparation
C <sub>3</sub> H <sub>9</sub> F <sub>6</sub> NS*	(CH <sub>3</sub> ) <sub>3</sub> N...SF <sub>6</sub>	D. Bittner	Spectrum assigned
C <sub>3</sub> H <sub>5</sub> NOS	C <sub>3</sub> H <sub>3</sub> NS...H <sub>2</sub> O (thiazole-water complex)	E. Gougoula	Spectra of isotopologues assigned
C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S	C <sub>3</sub> H <sub>3</sub> NS...(H <sub>2</sub> O) <sub>2</sub> (thiazole-(water) <sub>2</sub> complex; 2 isomers)	E. Gougoula	Spectra of isotopologues assigned
C <sub>3</sub> H <sub>9</sub> NO <sub>3</sub> S	C <sub>3</sub> H <sub>3</sub> NS...(H <sub>2</sub> O) <sub>2</sub> (thiazole-(water) <sub>3</sub> complex)	E. Gougoula	Tentative assignment
C <sub>4</sub> H <sub>3</sub> BrN <sub>2</sub>	5-bromopyrimidine	E. Gougoula	Spectrum assigned
C <sub>4</sub> H <sub>3</sub> ClN <sub>2</sub>	2-chloropyrimidine	E. Gougoula	Spectrum assigned
C <sub>4</sub> H <sub>5</sub> N <sub>3</sub>	2-aminopyrimidine	E. Gougoula	Spectrum assigned
C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	2-methyl-4(5)-nitroimidazole	E. Gougoula	Spectrum assigned
C <sub>4</sub> H <sub>6</sub> ArN <sub>2</sub>	1-methylimidazole-argon complex	C. Medcraft, J. Heitkämper, E. Gougoula	Manuscript in preparation
C <sub>4</sub> H <sub>6</sub> Ar <sub>2</sub> N <sub>2</sub>	1-methylimidazole-(argon) <sub>2</sub> complex	E. Gougoula, R. Paget	Spectrum assigned
C <sub>4</sub> H <sub>6</sub> ArN <sub>2</sub>	2-methylimidazole-argon complex	E. Gougoula, C. Medcraft	Manuscript in preparation
C <sub>4</sub> H <sub>6</sub> ArN <sub>2</sub>	4-methylimidazole-argon complex	E. Gougoula, C. Medcraft	Manuscript in preparation.
C <sub>4</sub> H <sub>6</sub> ArN <sub>2</sub>	5-methylimidazole-argon complex	E. Gougoula, C. Medcraft	Manuscript in preparation
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub>	1-methylimidazole	E. Gougoula, C. Medcraft	J. Chem. Phys. <b>151</b> , 144301 (2019)
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub>	2-methylimidazole	C. Medcraft, J. Heitkämper, E. Gougoula	J. Chem. Phys. <b>151</b> , 144301 (2019)
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub>	4-methylimidazole	E. Gougoula, C. Medcraft	J. Chem. Phys. <b>151</b> , 144301 (2019)
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub>	5-methylimidazole	E. Gougoula, C. Medcraft	J. Chem. Phys. <b>151</b> , 144301 (2019)
C <sub>4</sub> H <sub>6</sub> O	Crotonaldehyde (2-butenal; 3 conformers)	C. Medcraft, E. Gougoula	Manuscript in preparation
C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> S	Thiamazole (methimazole)	E. Gougoula, C. Lacey	Spectra of isotopologues assigned.
C <sub>4</sub> H <sub>6</sub> ArN <sub>2</sub> S	Thiamazole-argon complex	E. Gougoula, C. Lacey	Spectrum assigned
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O	1-methylimidazole-water complex	C. Medcraft, J. Heitkämper, E. Gougoula	Spectra of isotopologues assigned

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	1-methylimidazole-(water) <sub>2</sub> complex	E. Gougoula, R. Paget	Spectrum assigned. Isotopic work in progress
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O	2-methylimidazole-water complex	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O	4-methylimidazole-water complex	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O	5-methylimidazole-water complex	E. Gougoula, C. Medcraft	Spectra of isotopologues assigned.
C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> OS	Thiamazole-water complex	E. Gougoula, C. Lacey	Spectra of isotopologues assigned
C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O*	CH <sub>4</sub> N <sub>2</sub> O...C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> (urea-imidazole complex)	S. Blanco (Valladolid), J.C. Mullaney, C. Medcraft,	Spectrum assigned, isotopic work.
C <sub>4</sub> H <sub>9</sub> NOS*	N(CH <sub>3</sub> ) <sub>3</sub> ...SCO	E. Gougoula, J. A. Moxon	Chem. Phys. Lett. <b>743</b> , 137177 (2020)
C <sub>4</sub> H <sub>9</sub> NS <sub>2</sub> *	N(CH <sub>3</sub> ) <sub>3</sub> ...CS <sub>2</sub>	E. Gougoula, C. Medcraft	Manuscript in preparation
C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	<i>Trans</i> -urocanic acid (4-imidazoleacrylic acid)	G. Cooper, C. Medcraft, E. Gougoula	Phys.Chem.Chem.Phys, <b>21</b> , 9495 (2019)
C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	<i>Trans</i> -urocanic Acid-water complex	G. Cooper, C. Medcraft, E. Gougoula	Spectrum assigned, isotopic work in progress
C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>	Tetrahydrofuran-acetic acid complex	D.P. Zaleski, A. King	Spectrum assigned, isotopic work in progress.
C <sub>8</sub> H <sub>9</sub> N <sub>3</sub>	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ...C <sub>5</sub> H <sub>5</sub> N (imidazole-pyridine complex)	E. Gougoula, R. Paget	Spectrum assigned, isotopic work in progress
C <sub>9</sub> N <sub>2</sub> H <sub>8</sub>	2-phenylimidazole	E. Gougoula	Spectrum assigned
CClPt*	FCPtCl	D. Bittner, G. Cooper, C. Medcraft	Spectra of isotopologues assigned.
CF <sub>2</sub> 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 <sub>3</sub> IN*	H <sub>3</sub> N...Au-I	D. Bittner, S.L. Stephens	Spectrum assigned.
FIPt*	FPtI	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>
<b>C<sub>2</sub>H<sub>2</sub>O<sub>3</sub></b> <b>(H(C=O)-)<sub>2</sub>O</b>	formic acid anhydride	A. Walters <sup>1</sup> , J.-C. Guillemin <sup>2</sup> , H. S. P. Müller <sup>3</sup> <i>et al</i>	Measurements and analysis started of ground state and some vibrational states. Presently 70-120 GHz, $v=0$ , $v_{11}=1$ , $v_{14}=1$ , $v_{15}=1,2,3,4,5$ . To be extended. 37-505 GHz.
<b>C<sub>4</sub>H<sub>7</sub>N</b> <b>(<i>n</i>-C<sub>3</sub>H<sub>7</sub>CN)</b>	<i>n</i> -propyl cyanide	A. Walters <sup>1</sup> , H. S. P. Müller <sup>3</sup> <i>et al</i>	Search for higher vibrational states of <i>anti</i> and <i>gauche</i> conformers.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_3H_4O_3$ ( $CH_3COCOOH$ )	Pyruvic Acid	Susanna Widicus Weaver Connor Wright Alec Kroll <sup>5</sup>	Submm spectrum acquired, assignment in progress
$CH_5N$ ( $CH_3NH_2$ )	Methylamine	Susanna Widicus Weaver Alec Kroll <sup>5</sup> Nathan Harper Connor Wright	Submm spectrum acquired, assignment in progress
$CH_4N^{\cdot}$ ( $CH_2NH_2^{\cdot}$ )	Aminomethyl Radical	Susanna Widicus Weaver Connor Wright John Stanton <sup>6</sup>	Submm spectrum acquisition and assignment in progress
$CH_5NO$ ( $HOCH_2NH_2$ )	Aminomethanol	Susanna Widicus Weaver Hayley Bunn Chase Schultz Brian Hays <sup>1</sup>	Submm spectrum acquisition and assignment in progress
EXPERIMENTAL	Millimeter/Submillimeter Spectroscopic Detection of Desorbed Ices: A New Technique in Laboratory Astrochemistry	Susanna Widicus Weaver Katarina Yocum Stefanie Milam <sup>4</sup> Houston H. Smith Ethan W. Todd Leslie Mora Perry A. Gerakines <sup>4</sup>	Published: <i>J. Phys. Chem. A</i> , 2019, 123(40), pp 8702-870
$CH_4ArO$ ( $Ar-H_3COH$ )	Argon Methanol Cluster	Susanna Widicus Weaver Kevin Roenitz	Submm spectrum acquisition and assignment in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_2H_4O_3$ ( $CH_3COCO_2H$ )	Glycolic Acid	Susanna Widicus Weaver Hayley Bunn Chase Schultz	Submm spectrum acquisition and assignment in progress
$C_2H_5NO_2$ ( $HOCH_2CONH_2$ )	Glycolamide	Susanna Widicus Weaver Hayley Bunn Chase Schultz	Submm spectrum acquisition and assignment 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>
CHN (HCN)	hydrogen cyanide	F. Rohart <sup>1</sup>	lineshape analysis in progress  Manuscript in preparation
CHN H <sup>15</sup> NC; H <sup>15</sup> N <sup>13</sup> C D <sup>15</sup> NC; D <sup>15</sup> N <sup>13</sup> C; H <sup>14</sup> N <sup>13</sup> C; D <sup>14</sup> N <sup>13</sup> C	hydrogen isocyanide	S. Bailleux <sup>1</sup> , P. Kania <sup>13</sup> , G. Wlodarczak <sup>1</sup>	spectrum assigned (mm+THz)  Manuscript in preparation
CH <sub>2</sub> CHD, CD <sub>2</sub>	methylene radical	S. Bailleux <sup>1</sup> , H. Ozeki <sup>14</sup>	spectrum assigned (THz) Manuscript in preparation
C <sub>2</sub> H <sub>3</sub> N (CH <sub>3</sub> CN)	methyl cyanide	F. Rohart <sup>1</sup> L. Zu <sup>1</sup> L. Margulès <sup>1</sup> R.A. Motiyenko <sup>1</sup>	Lineshape analysis in progress
CH <sub>3</sub> NO (CH <sub>3</sub> NO)	nitrosomethane	L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup>	MM spectra+SMM spectra; internal rotation  Analysis in progress
CH <sub>3</sub> NO (CH <sub>2</sub> NOH)	formaldoxime	L. Zou <sup>1</sup> L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup>	MM spectra+SMM spectra;  Analysis in progress
CH <sub>3</sub> NS (NH <sub>2</sub> CHS)	thioformamide	R. A. Motiyenko <sup>1</sup> L. Margulès <sup>1</sup> , J.-C. Guillemin <sup>2</sup>	MM spectra+SMM spectra;  Manuscript in preparation



<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
CH <sub>4</sub> O (CHD <sub>2</sub> OH)	methanol	L. Coudert <sup>6</sup> , L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup>	MM+SMM+THz spectra; internal rotation Analysis in progress
C <sub>2</sub> H <sub>3</sub> NO (HO <sup>13</sup> CH <sub>2</sub> CN, HOCH <sub>2</sub> <sup>13</sup> CN, DOCH <sub>2</sub> CN)	hydroxy-acetonitrile	L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup>	MM spectra+SMM spectra; tunnelling  Analysis in progress
C <sub>2</sub> H <sub>3</sub> NO <sub>2</sub> (H <sub>3</sub> ONCO)	methoxy-isocyanate	A. Pienkina <sup>1</sup> L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup> J. Cernicharo <sup>4</sup>	MM spectra  Manuscript in preparation
C <sub>2</sub> H <sub>4</sub> O (CH <sub>2</sub> DCHO)	acetaldehyde	L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup> L. Coudert <sup>7</sup>	MM+SMM spectra; internal rotation A&A 624, A70 (2019) <a href="https://doi.org/10.1051/0004-6361/201834827">https://doi.org/10.1051/0004-6361/201834827</a>
C <sub>2</sub> H <sub>4</sub> S (CH <sub>3</sub> CHS)	thioacetaldehyde	L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup> V. Illyushin <sup>3</sup>	MM spectra+SMM spectra;  J. Mol. Spectrosc. Accepted
C <sub>2</sub> H <sub>5</sub> N (CH <sub>3</sub> CHNH)	ethaneimine	L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup> B. Mc Guirre <sup>8</sup> A. Remijan <sup>8</sup>	MM spectra internal rotation  Manuscript in preparation
C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub> (CH <sub>3</sub> CONCO)	acetyl-isocyanate	L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup> I. Kleiner <sup>7</sup> V. Illyushin <sup>3</sup> J. Cernicharo <sup>4</sup>	MM spectra internal rotation  Analysis in progress
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> (CH <sub>3</sub> N-CH-CN)	methylimino-acetonitrile	R. A. Motiyenko <sup>1</sup> L. Margulès <sup>1</sup> , J.-C. Guillemin <sup>2</sup>	MM spectra internal rotation  Analysis in progress
C <sub>3</sub> H <sub>4</sub> O <sub>4</sub>	Malonic acid	W. Chin <sup>6</sup> , M. Goubet <sup>1</sup>	Experiments and Analyses in progress

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>3</sub> H <sub>5</sub> N ( <sup>13</sup> C-CH <sub>3</sub> CH <sub>2</sub> CN)	ethyl cyanide	J. Pearson <sup>9</sup> B. Drouin <sup>9</sup> Y. ShanShan <sup>9</sup> L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup>	MM+SMM+THz spectra exc. states  Analysis in progress
C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> COOH)	propionic acid	A. Kutsenko <sup>3</sup> V. Illyushin <sup>3</sup> R. A. Motiyenko <sup>1</sup> L. Margulès <sup>1</sup> , J.L. Alonso <sup>5</sup> J. Cernicharo <sup>4</sup>	MM+SMM spectra; internal rotation  Manuscript in preparation
C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> (C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> ... H <sub>2</sub> O)	Methylglyoxal hydrate	S. Bteich <sup>1</sup> , M. Goubet <sup>1</sup> , T.R. Huet <sup>1</sup>	Experiments Completed  Analyses in progress
C <sub>3</sub> H <sub>7</sub> N (CH <sub>3</sub> CH <sub>2</sub> CHNH)	propaneimine	L. Margulès <sup>1</sup> , R. A. Motiyenko <sup>1</sup> J.-C. Guillemin <sup>2</sup> B. Mc Guirre <sup>8</sup> A. Remijan <sup>8</sup>	MM+SMM spectra  Manuscript in preparation
C <sub>3</sub> H <sub>7</sub> NO (CH <sub>3</sub> CH <sub>2</sub> CONH <sub>2</sub> )	propionamide	V. Illyushin <sup>3</sup> E. Alekseev <sup>3</sup> R. A. Motiyenko <sup>1</sup> L. Margulès <sup>1</sup> P. Drean <sup>1</sup>	MW+MM+SMM spectra; internal rotation  Analysis in progress
C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>	Succinic acid	W. Chin <sup>6</sup> , M. Goubet <sup>1</sup>	Experiments and Analyses in progress
C <sub>5</sub> H <sub>8</sub> N <sub>2</sub>	2-cyanopyrrolidine	R. A. Motiyenko <sup>1</sup> L. Margulès <sup>1</sup> , J.-C. Guillemin <sup>2</sup> S. Samdal <sup>10</sup>	MM spectra  Analysis in progress
C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	2-Nitrotoluene 4-Nitrotoluene	A. Roucou <sup>11</sup> , I. Kleiner <sup>7</sup> , M. Goubet <sup>1</sup> S. Bteich <sup>1</sup> , A. Cuisset <sup>11</sup>	Experiments and analyses completed Manuscript in preparation

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>10</sub> H <sub>8</sub> O	1-hydroxynaphthalene 2-hydroxynaphthalene	O. Pirali <sup>6</sup> , M-A Martin-Drumel <sup>6</sup> , M. Goubet <sup>1</sup> , F. Réal <sup>1</sup> , V. Vallet <sup>1</sup>	Manuscript under revision (JPCA)
C <sub>11</sub> H <sub>8</sub> O	1-naphthaldehyde 2-naphthaldehyde	O. Pirali <sup>6</sup> , M-A Martin-Drumel <sup>6</sup> , M. Goubet <sup>1</sup> , F. Réal <sup>1</sup> , V. Vallet <sup>1</sup>	Manuscript under revision (JPCA)
C <sub>10</sub> H <sub>16</sub> O	2-adamantanol	O. Pirali <sup>6</sup> , M-A Martin-Drumel <sup>6</sup> , O. Chitarra <sup>6</sup> , M. Goubet <sup>1</sup> , J. Claus <sup>1</sup>	Experiments and analyses in progress
H <sub>2</sub> S	hydrogen disulfide	F. Rohart <sup>1</sup> A. Cuisset <sup>11</sup> M. Mouelhi <sup>11,12</sup> H. Aroui <sup>12</sup> et al.	lineshape analysis (MM+THz)  Accepted manuscript
<sup>14</sup> NO <sup>+</sup> <sup>15</sup> NO <sup>+</sup>	nitrosylium ion	S. Bailleux <sup>1</sup> E. Alekseev <sup>3</sup> J. Cernicharo <sup>4</sup>	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 <sub>10</sub> H <sub>18</sub> O <sub>2</sub> (C <sub>10</sub> H <sub>16</sub> O-H <sub>2</sub> O)	Perillyl alcohol-water	F. Xie	Conformational search done; Monohydrate assignment in progress.
C <sub>10</sub> H <sub>16</sub> O <sub>6</sub> ((C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> ) <sub>2</sub> )	Tetrahydro-2-furoic acid dimer	F. Xie <sup>1</sup> N. Seifert	Angew. Chem. Int. Ed. 2020; <a href="https://doi.org/10.1002/anie.202005685">https://doi.org/10.1002/anie.202005685</a> .
C <sub>5</sub> H <sub>10</sub> O <sub>4</sub> (C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> -H <sub>2</sub> O)	Tetrahydro-2-furoic acid -water	F. Xie, <sup>1</sup> S. Mahendiran	Several conformers assigned; MS near completion.
C <sub>8</sub> H <sub>14</sub> O <sub>4</sub> (C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> -C <sub>3</sub> H <sub>6</sub> O)	Tetrahydro-2-furoic acid -propylene oxide dimer	F. Xie	Several dimers assigned; MS near completion.
C <sub>9</sub> H <sub>18</sub> O <sub>3</sub> (C <sub>3</sub> H <sub>6</sub> O) <sub>3</sub>	Propylene oxide trimer	F. Xie, <sup>1,2</sup> A. Hazrah	Several conformers assigned; MS near completion.
C <sub>12</sub> H <sub>24</sub> O <sub>4</sub> (C <sub>3</sub> H <sub>6</sub> O) <sub>4</sub>	Propylene oxide tetramer	F. Xie	Several conformers assigned.
C <sub>10</sub> H <sub>12</sub> O <sub>6</sub> C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> -C <sub>5</sub> H <sub>4</sub> O <sub>3</sub>	Tetrahydro-2-furoic acid -2-furoic acid dimer	F. Xie	Several binary conformers assigned; MS in preparation.
C <sub>6</sub> H <sub>16</sub> O <sub>6</sub> ((C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> ) <sub>2</sub> )	Glycerol dimer (propane-1,2,3-triol) <sub>2</sub>	F. Xie <sup>1</sup> N. Seifert	Extensive conformational scans done; Several new dimers assigned.
C <sub>3</sub> H <sub>10</sub> O <sub>4</sub> C <sub>3</sub> H <sub>12</sub> O <sub>5</sub> C <sub>3</sub> H <sub>14</sub> O <sub>6</sub> (C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> -(H <sub>2</sub> O) <sub>1,2,3</sub> )	Glycerol-(H <sub>2</sub> O) <sub>1,2,3</sub> Clusters	F. Xie J. Thomas	Extensive conformational scans done; Assignment in progress.
C <sub>6</sub> H <sub>10</sub> F <sub>6</sub> O <sub>2</sub> (C <sub>3</sub> H <sub>5</sub> F <sub>3</sub> O) <sub>2</sub>	3,3,3-trifluoropropanol (TFP) dimer	F. Xie N. Seifert	One new monomer and three dimers assigned; MS in preparation.
C <sub>3</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> (C <sub>3</sub> H <sub>5</sub> F <sub>3</sub> O-H <sub>2</sub> O)	TFP-H <sub>2</sub> O	F. Xie	Conformational search completed; Assignment in progress.
C <sub>7</sub> H <sub>10</sub> F <sub>6</sub> O <sub>3</sub> (C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> )	1,1,1,3,3,3- hexafluoro -2-propanol (HFIP)-1,4-dioxane	F. Xie, N. Bui, Q. Yang	Spectra assigned; MS in preparation.
C <sub>12</sub> H <sub>15</sub> F <sub>3</sub> O <sub>3</sub> (C <sub>8</sub> F <sub>3</sub> H <sub>7</sub> O-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> )	1-phenyl-2,2,2-trifluoro ethanol-1,4-dioxane	Q. Yang, F. Xie	Assignment in progress.
C <sub>6</sub> H <sub>11</sub> F <sub>3</sub> O <sub>3</sub> (C <sub>2</sub> F <sub>3</sub> H <sub>3</sub> O-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> )	2, 2, 2-trifluoroethanol (TFE)-1,4-dioxane	Q. Yang	Assignment in progress.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>8</sub> H <sub>14</sub> F <sub>6</sub> O <sub>2</sub> (C <sub>4</sub> H <sub>7</sub> F <sub>3</sub> O) <sub>2</sub>	4,4,4-trifluorobutanol (TFB) dimer	T. Lu, F. Xie <sup>1</sup>	Conformational search completed; One dimer assigned; others in progress.
C <sub>4</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub> (C <sub>4</sub> H <sub>7</sub> F <sub>3</sub> O-H <sub>2</sub> O)	TFB-H <sub>2</sub> O	T. Lu, F. Xie <sup>1</sup>	Conformational search completed; Assignment in progress.
C <sub>4</sub> H <sub>7</sub> NO (C <sub>4</sub> H <sub>5</sub> N-(H <sub>2</sub> O)) C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> (C <sub>4</sub> H <sub>5</sub> N-(H <sub>2</sub> O) <sub>2</sub> )	Pyrrole-(water) <sub>1,2</sub>	B. Wu F. Xie, J. Thomas	New conformational and TS calculations; <sup>13</sup> C of Py-1W assigned; search for Py-2W completed; MS near completion.
C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> N <sub>2</sub> O (C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O-N <sub>2</sub> )	1,1,1,3,3,3- hexafluoro -2-propanol (HFIP) with N <sub>2</sub>	S. Oswald <sup>1,3</sup> N. Seifert B. Wu	Spectra assigned; <sup>14</sup> N hfs analysis completed; MS near completion.
C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> NeO (C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O-Ne) C <sub>3</sub> H <sub>2</sub> ArF <sub>6</sub> O (C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O-Ar)	1,1,1,3,3,3- hexafluoro -2-propanol (HFIP) with Ne and with Ar	B. Wu <sup>1</sup> S. Oswald N. Seifert	Spectra assigned; MS near completion.
C <sub>3</sub> H <sub>4</sub> F <sub>6</sub> O <sub>2</sub> (C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O-H <sub>2</sub> O)	HFIP-H <sub>2</sub> O	B. Wu, N. Seifert S. Oswald	A new conformer assigned. HOD, DOH and D <sub>2</sub> O analysis completed. MS in preparation.
C <sub>3</sub> H <sub>3</sub> F <sub>5</sub> O C <sub>3</sub> H <sub>3</sub> F <sub>5</sub> NeO (C <sub>3</sub> H <sub>3</sub> F <sub>5</sub> O-Ne)	2,2,3,3,3-pentafluoro -1-propanol (PFP) monomer and with Ne	B. Wu <sup>1</sup> S. Oswald N. Seifert	One monomer fitted; Tunneling splitting observed; Detailed fits in progress
C <sub>6</sub> H <sub>6</sub> F <sub>10</sub> O <sub>2</sub> ((C <sub>3</sub> H <sub>3</sub> F <sub>5</sub> O) <sub>2</sub> )	PFP dimer	S. Oswald <sup>1,3</sup> B. Wu, N. Seifert	Five dimers assigned; MS in preparation.
C <sub>3</sub> H <sub>5</sub> F <sub>5</sub> O <sub>2</sub> (C <sub>3</sub> H <sub>3</sub> F <sub>5</sub> O-H <sub>2</sub> O)	PFP-H <sub>2</sub> O	B. Wu, N. Seifert S. Oswald	Two conformers assigned; HOD, DOH and D <sub>2</sub> O analysis completed; MS in preparation.
C <sub>8</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub> (C <sub>8</sub> F <sub>3</sub> H <sub>7</sub> O-H <sub>2</sub> O)	1-phenyl-2,2,2- trifluoroethanol-water	C Carlson, D. Mason N. Seifert	Monohydrate and isotopologues assigned; MS near completion.
C <sub>16</sub> H <sub>14</sub> F <sub>6</sub> O <sub>2</sub> (C <sub>8</sub> F <sub>3</sub> H <sub>7</sub> O) <sub>2</sub>	1-phenyl-2,2,2- Trifluoroethanol dimer	C. Carlson N. Seifert	Assignment in progress.
C <sub>2</sub> F <sub>3</sub> H <sub>6</sub> NO (C <sub>2</sub> F <sub>3</sub> H <sub>3</sub> O-NH <sub>3</sub> )	Trifluoroethanol -ammonia	J. Thomas, <sup>1</sup> I. Peña <sup>4</sup> C. Carlson, Y. Yang	MS near completion.
C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> -H <sub>2</sub> O	Cyclohexanecarboxylic acid and its hydrates	T. Lu, <sup>1,5</sup> A. S. Hazrah F.Xie	One conformer assigned for monomer; others in progress.
C <sub>6</sub> H <sub>6</sub> F <sub>6</sub> O <sub>2</sub> ((C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O) <sub>2</sub> )	Trifluoromethyl oxirane dimer	H. O. Leung <sup>1,6</sup> M. D. Marshall N. Seifert	Spectra assigned; MS in preparation.
C <sub>9</sub> H <sub>18</sub> O <sub>4</sub> (C <sub>6</sub> H <sub>12</sub> O <sub>3</sub> -C <sub>3</sub> H <sub>6</sub> O)	Solketal-propylene oxide complex	L. Evangelisti, J. Thomas, C. West <sup>7</sup>	Spectra assigned; MS in preparation.

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
$C_8H_{12}F_{12}O_4$ $((C_2H_3F_3O)_4)$	(Trifluoroethanol) <sub>4</sub>	J. Thomas <sup>1</sup> N. Seifert	Extensive conformational search (TFE) <sub>4</sub> assignment in progress.
$C_8H_{11}NO_3$ $(C_8H_8O_3-NH_3)$	Methyl salicylate -ammonia	J. Thomas <sup>1</sup>	New conformers predicted; chirped and cavity assignments in progress.
$C_2H_7FO_2$ $C_2H_9FO_3$ $C_2H_{11}FO_4$ $(C_2H_5FO-(H_2O)_{1-3})$	2-fluoroethanol -(water) <sub>n</sub>	W. Huang J. Thomas	Extensive theoretical calculations for n up to 3; broadband spectra recorded; assignment in progress.
$C_4H_{10}O_5$ $C_4H_{12}O_6$ $(C_4H_6O_3-(H_2O)_{2-3})$	Methyl glycidate -(water) <sub>2-3</sub>	J. Thomas, Z. Wang	Theoretical calculation with n up to 3; broadband spectra recorded and assignment of others in progress.
$C_4H_9NO_3$ $(C_4H_6O_3-NH_3)$	Methyl glycidate -ammonia	J. Thomas	Broadband spectra recorded and assigned; hfs analysis with cavity measurement in progress.
$C_8H_{16}O_6$ $(C_4H_8O_3-C_4H_8O_3)$	Methyl lactate dimers	J. Thomas N. Seifert	Extensive ab initio conformational search completed; broadband spectra recorded; assignment in progress.
$C_3H_{12}O_4$ $C_3H_{14}O_5$ $(C_3H_6O-(H_2O)_{3,4})$	Propylene oxide -(water) <sub>n</sub>	J. Thomas Z. Su	Extensive calculations with n=3 and 4 broadband and cavity spectra recorded; n=3 assigned and n=4 in progress.
$C_3H_5FO_2$	$\alpha$ -Fluoropropionic acid	Y. Yang J. Thomas	New measurements and theoretical study
$CH_6O$ $(CH_4-H_2O)$	Methane-water	X. Liu	IR spectrum at H <sub>2</sub> O $\nu_2$ band measured; assignment in progress.
$H_3NNe$ $(Ne-NH_3)$	Ammonia-neon,	X. Liu	IR spectrum at NH <sub>3</sub> $\nu_4$ band assigned.
$ArH_3N$ $(Ar-NH_3)$	Ammonia-argon,	X. Liu	IR spectrum at NH <sub>3</sub> $\nu_4$ band assigned.
$C_3H_8O_2$ $(C_3H_6O-H_2O)$	Propylene oxide -water	J. Thomas X. Liu R. Patel	Rich IR spectrum at H <sub>2</sub> O $\nu_2$ band measured; assignment in progress.
$CH_3NO$ $(HCONH_2)$	Formamide	F. Sunahori	High-res. IR Spectra obtained; assigned
$C_2H_6N_2O_2$ $((HCONH_2)_2)$	Formamide dimer	F. Sunahori	High-res. IR Spectra obtained; assignment in progress.
$C_4H_8O_3$	Methyl lactate	F. Sunahori N. Borho	High-res. IR spectrum obtained; assignment in slow progress.

- <sup>1</sup> In collaboration with Prof. W. Jäger, Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada, T6G 2G2.
- <sup>2</sup> In collaboration with Dr. M. Fusè and Prof. V. Barone, Scuola Normale Superiore, Piazza dei Cavalieri 7 56126 Pisa, Italy.
- <sup>3</sup> In collaboration with Prof. M. Suhm, University of Göttingen, Institute of Physical Chemistry, Tammannstraße 6 D-37077 Göttingen, Germany.
- <sup>4</sup> In collaboration with Dr. I. I. Peña, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid, Spain.
- <sup>5</sup> In collaboration with Prof. Q. Gou and G. Feng, School of Chemistry and Chemical Engineering, Chongqing University, Daxuecheng South Rd. 55, 401331, Chongqing, China.
- <sup>6</sup> In collaboration with Prof. H. O. Leung and Prof. M. D. Marshall, Department of Chemistry, Amherst College P.O. Box 5000, Amherst, MA 01002-5000.
- <sup>7</sup> In collaboration with Prof. W. Caminati, University of Bologna and Prof. B. H. Pate, University of Virginia.



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Formula	Name of Compound	Name of Investigator	Present Stage of Progress
KO	Potassium Oxide	Burton et al.	<i>PCCP</i> , <b>21</b> , 21960 (2019)
BrCr	Chromium Bromide	Herman & Ziurys	<i>JCP</i> , <b>151</b> , 194301 (2019)
CH <sub>3</sub> ClZn	Methyl Zinc Chloride	Burton, Tabassum & Ziurys	<i>JMS</i> , <b>386</b> , 111256 (2020)
<sup>13</sup> C <sub>2</sub> Sc, <sup>12</sup> C <sup>13</sup> CSc	Scandium Dicarbide	Burton et al.	<i>JCP</i> , under review
PSi	Silicon Phosphide	Burton & Ziurys	Manuscript in prep.
BrTi	Titanium Bromide	Herman, Tabassum & Ziurys	Spectrum under analysis

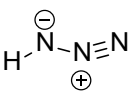
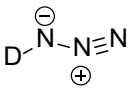
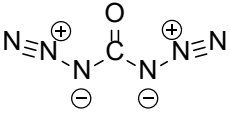
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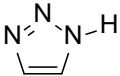
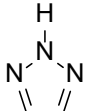





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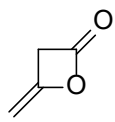
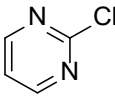
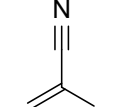
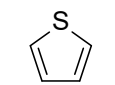
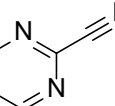
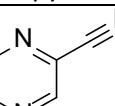
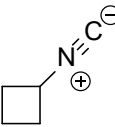
FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR(S)	PRESENT STAGE OF PROGRESS
HN <sub>3</sub>	 hydrazoic acid	V. L. Orr B. K. Amberger B. J. Esselman S. Urban <sup>1</sup> K. Vavra <sup>1</sup> Z. Kisiel <sup>2</sup> R. C. Woods R. J. McMahon	8 - 700+ GHz spectrum obtained Fitting and assignment of vibrational states underway
DN <sub>3</sub>	 deuteriohydrazoic acid	V. L. Orr B. K. Amberger B. J. Esselman S. Urban <sup>1</sup> K. Vavra <sup>1</sup> Z. Kisiel <sup>2</sup> R. C. Woods R. J. McMahon	130 - 375 GHz spectrum obtained Fitting and assignment of vibrational states underway
CHN	H-C≡N hydrogen cyanide	H. E. Warner B. J. Esselman J. F. Stanton <sup>3</sup> R. C. Woods R. J. McMahon	HCN measured in multiple isotopologues Experimental alpha, gamma, and epsilon vibration-rotation interactions determined
CN <sub>6</sub> O	 carbonyl diazide	P. M. Dorman B. K. Amberger B. J. Esselman R. C. Woods R. J. McMahon	235 – 375 GHz spectrum obtained <i>J. Mol. Spectrosc.</i> <b>2014</b> , 295, 15-20. Fitting of a coupled tetrad underway

<sup>1</sup> University of Chemistry and Technology, Prague


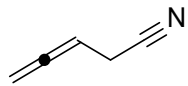
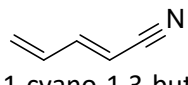
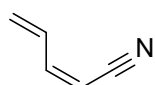
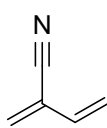
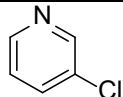
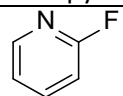
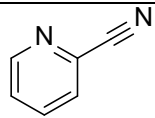
<sup>2</sup> Institute of Physics, Polish Academy of Sciences

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR(S)	PRESENT STAGE OF PROGRESS
C <sub>2</sub> H <sub>3</sub> N <sub>3</sub>	 1H-1,2,3-triazole	M. A. Zdanovskaia B. J. Esselman S. M. Kougias J. F. Stanton <sup>3</sup> R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained $r_e^{SE}$ structure determination underway Spectra of several isotopologues obtained Spectra of several vibrationally excited states fit
C <sub>2</sub> H <sub>3</sub> N <sub>3</sub>	 2H-1,2,3-triazole	M. A. Zdanovskaia B. J. Esselman S. M. Kougias J. F. Stanton <sup>3</sup> R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained $r_e^{SE}$ structure determination underway Spectra of several isotopologues obtained Spectra of several vibrationally excited states fit
C <sub>3</sub> H <sub>3</sub> NO	 isoxazole	M. D. Fellows B. J. Esselman N. Horinouchi <sup>4</sup> K. Kobayashi <sup>4</sup> R. C. Woods R. J. McMahon	130 – 360 GHz spectrum obtained Spectra of several isotopologues obtained Spectra of several vibrationally excited states fit obtained Synthesis of deuterated isotopologues and $r_e^{SE}$ structure determination underway.
C <sub>3</sub> H <sub>3</sub> NS	 1,3-thiazole	B. J. Esselman M. A. Zdanovskaia L. S. Sowin R. C. Woods R. J. McMahon	130 – 230 GHz spectrum obtained Fit of GS complete Fitting of vibrationally excited states and isotopologues underway. Synthesis of deuterated isotopologues and $r_e^{SE}$ structure determination underway
C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	 pyrazole	M. A. Zdanovskaia B. J. Esselman R. C. Woods R. J. McMahon	Accidentally obtained in commercial sample of triazole 235 – 360 GHz spectrum obtained Fitting of GS complete
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	 pyridazine	M. A. Zdanovskaia B. J. Esselman B. K. Amberger R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of GS and effective fits of vibrationally excited states complete <i>J. Chem. Phys.</i> <b>2013</b> , 139, 224304 Fit of coupled dyad underway Additional vibrational satellite fit
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	 pyrimidine	Z. N. Heim <sup>5</sup> B. K. Amberger B. J. Esselman J. F. Stanton <sup>3</sup> R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained $r_e^{SE}$ structure from many isotopologues <i>J. Chem. Phys.</i> <b>2020</b> , manuscript accepted Several vibrationally excited states fit

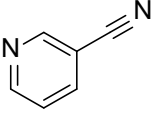
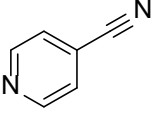
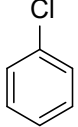
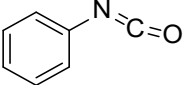
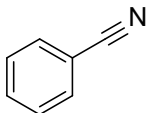
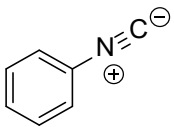
<sup>3</sup> University of Florida<sup>4</sup> University of Toyama<sup>5</sup> University of California

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR(S)	PRESENT STAGE OF PROGRESS
C <sub>4</sub> H <sub>4</sub> O <sub>2</sub>	 diketene	V. L. Orr B. J. Esselman P. M. Dorman R. C. Woods R. J. McMahon	235 – 375 GHz spectrum obtained <i>J. Phys. Chem. A</i> <b>2016</b> , <i>120</i> , 7753-7763 Fitting of a coupled dyad underway
C <sub>4</sub> H <sub>3</sub> ClN <sub>2</sub>	 2-chloropyrimidine	N. Love <sup>6</sup> K. Belmont <sup>6</sup> K. R. Leopold <sup>6</sup> B. J. Esselman R. C. Woods R. J. McMahon	130 – 360 GHz spectrum obtained Fitting of <sup>35/37</sup> Cl GS and several vibrational states underway
C <sub>4</sub> H <sub>5</sub> N	 methacrylonitrile	H. H. Smith S. M. Kougiias D. J. Lee B. J. Esselman R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of GS complete with methyl rotor Fitting of vibrationally excited states underway Synthesis of methacrylonitrile-d <sub>n</sub> complete Fitting of over a dozen isotopologues complete, r <sub>e</sub> <sup>SE</sup> structure determination underway
C <sub>4</sub> H <sub>4</sub> S	 thiophene	V. L. Orr Y. Ichikawa <sup>4</sup> A. R. Patel S. M. Kougiias K. Kobayashi <sup>4</sup> B. J. Esselman R. C. Woods R. J. McMahon	130 – 360 GHz spectrum obtained Fitting of GS and several vibrational states underway Preparation of all thiophenes-d <sub>n</sub> complete, fitting underway. r <sub>e</sub> <sup>SE</sup> structure determination underway
C <sub>5</sub> H <sub>3</sub> N <sub>3</sub>	 cyanopyrimidine	H. H. Smith B. J. Esselman R. C. Woods R. J. McMahon	130 – 360 GHz spectrum obtained Spectra of ground state fit Analysis of dyad of 1 <sup>st</sup> and 2 <sup>nd</sup> fundamental underway
C <sub>5</sub> H <sub>3</sub> N <sub>3</sub>	 cyanopyrazine	B. J. Esselman R. C. Woods R. J. McMahon	130 – 360 GHz spectrum obtained Spectra of ground state fit Analysis of dyad of 1 <sup>st</sup> and 2 <sup>nd</sup> fundamental underway
C <sub>5</sub> H <sub>7</sub>	 cyclobutylisocyanide	M. D. Fellows S. M. Kougiias B. J. Esselman R. C. Woods R. J. McMahon	235 – 360 GHz spectrum obtained Spectra of equatorial conformation obtained. Spectra of several vibrationally excited states fit obtained

<sup>6</sup> University of Minnesota

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR(S)	PRESENT STAGE OF PROGRESS
C <sub>5</sub> H <sub>5</sub> N	 pyridine	M. A. Zdanovskaia B. J. Esselman J. F. Stanton <sup>3</sup> R. C. Woods R. J. McMahon	130 – 360 GHz spectrum obtained Fit of ground state and vibrationally excited states underway Pyridine- <i>d</i> <sub>2</sub> synthesized and pyridine- <i>d</i> <sub>5</sub> obtained Fits of deuterio-isotopologues underway
C <sub>5</sub> H <sub>5</sub> N	 4-cyano-1,2-butadiene	V. L. Orr S. M. Kougiass B. J. Esselman R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of syn and anti GS and vibrationally excited states underway.
C <sub>5</sub> H <sub>5</sub> N	 <i>E</i> -1-cyano-1,3-butadiene	M. A. Zdanovskaia S. M. Kougiass B. J. Esselman R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained GS effective fit obtained Fitting of GS and vibrationally excited states underway.
C <sub>5</sub> H <sub>5</sub> N	 <i>Z</i> -1-cyano-1,3-butadiene	K. Lee <sup>7</sup> M. C. McCarthy <sup>7</sup> P. M. Dorman S. M. Kougiass B. J. Esselman R. C. Woods R. J. McMahon	8 – 20 GHz spectrum obtained 130 – 375 GHz spectrum obtained Fitting of GS complete with nuc quadrupole coupling. Fitting of couple dyad of the first and second fundamentals underway.
C <sub>5</sub> H <sub>5</sub> N	 2-cyano-1,3-butadiene	B. J. Esselman M. Zdanovskaia S. M. Kougiass D. J. Lee A. R. Patel R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of GS complete. Fitting of couple dyad of the first and second fundamentals underway.
C <sub>5</sub> H <sub>4</sub> ClN	 3-chloropyridine	B. J. Esselman R. C. Woods R. J. McMahon	130 – 360 GHz spectrum obtained Fitting of gs underway
C <sub>5</sub> H <sub>4</sub> FN	 2-fluoropyridine	B. J. Esselman R. C. Woods R. J. McMahon	235 – 360 GHz spectrum obtained Fitting of GS and several vibrational states underway
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	 2-cyanopyridine	P. M. Dorman B. J. Esselman R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of GS complete. Fitting of coupled dyad near-completion Presented at ISMS 2019

<sup>7</sup> Harvard-Smithsonian Center for Astrophysics

FORMULA	NAME OF COMPOUND	NAME OF INVESTIGATOR(S)	PRESENT STAGE OF PROGRESS
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	 3-cyanopyridine	P. M. Dorman B. J. Esselman R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of GS complete. Fitting of coupled dyad complete Manuscript in preparation.
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	 4-cyanopyridine	P. M. Dorman J. Park B. J. Esselman R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of GS complete. Fitting of coupled dyad complete Manuscript submitted to <i>J Mol Spec.</i>
C <sub>6</sub> H <sub>5</sub> Cl	 Chlorobenzene	B. J. Esselman R. C. Woods R. J. McMahon	130 – 360 GHz spectrum obtained Fitting of GS and several vibrational states underway
C <sub>7</sub> H <sub>5</sub> NO	 phenyl isocyanate	C. E. Schwarz B. J. Esselman B. K. Amberger R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of coupled tetrad of GS and first three vibrationally excited states underway
C <sub>7</sub> H <sub>5</sub> N	 Benzonitrile	M. A. Zdanovskaia Z. Kisiel <sup>2</sup> B. J. Esselman R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of ground state and coupled dyad complete <i>J. Mol. Spectrosc.</i> <b>2018</b> , 351, 39-48. Fitting of coupled triad underway
C <sub>7</sub> H <sub>5</sub> N	 Phenyl isocyanide	M. A. Zdanovskaia B. J. Esselman R. C. Woods R. J. McMahon	130 – 375 GHz spectrum obtained Fitting of ground state and coupled dyad complete Coupled tetrad observed and predicted <i>J. Chem. Phys.</i> <b>2019</b> , 151, 024301.

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<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>5</sub> H <sub>13</sub> NO	5-aminopentanol	R. Lavrich <sup>1</sup>	Two conformers of parent assigned; Searching for <sup>13</sup> C spectra
C <sub>4</sub> H <sub>11</sub> NO	1-amino-2-methyl-2-propanol	R. Lavrich <sup>1</sup> , G. Brown <sup>2</sup> , A.-M. Kelterer <sup>3</sup>	Manuscript in Preparation; Search for water complex underway
C <sub>4</sub> H <sub>5</sub> F <sub>6</sub> NO	1-amino-2,2-bis(trifluoromethyl)-2-ethanol	R. Lavrich <sup>1</sup> , G. Brown <sup>2</sup> , A.-M. Kelterer <sup>3</sup>	Manuscript in Preparation; Search for water complex underway
C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	Dimethylaminopyridine	R. Lavrich <sup>1</sup>	Parent assigned; <sup>15</sup> N experiments in progress; Search for water complex underway
C <sub>9</sub> H <sub>16</sub> O	2-nonenal	R. Lavrich <sup>1</sup>	Experiments in Progress
C <sub>14</sub> H <sub>10</sub> O <sub>2</sub>	9-hydroxy-5-methylphenalenone	R. Lavrich <sup>1</sup> , V. V. Ilyushin <sup>4</sup>	Experiments in Progress

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(Entries marked with ^ are collaborative studies between this laboratory and that of M.E. Sanz, Chemistry Department, Britannia House King's College London, SE1 1DB, UK)

<u>FORMULA</u>	<u>NAME OF COMPOUND</u>	<u>NAME OF INVESTIGATOR</u>	<u>PRESENT STAGE OF PROGRESS</u>
C <sub>4</sub> H <sub>6</sub> O*	2-butenal (crotonaldehyde)	C. Medcraft, E.Gougoula, N.R.Walker	Manuscript in preparation
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> *	2-butenal-water complex	C. Medcraft, E.Gougoula, N.R.Walker	Spectrum assigned
C <sub>2</sub> O <sub>2</sub> F <sub>3</sub> l*	CF <sub>3</sub> l---CO <sub>2</sub>	C. Medcraft, N.R.Walker	Manuscript in preparation
C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ^	Hinoikitiol, (b- thujaplicin)	C. Medcraft, S.I. Murugachandran, M.E. Sanz	Spectrum assigned
C <sub>10</sub> H <sub>14</sub> O <sub>3</sub> ^	Hinoikitiol – 1w	C. Medcraft, S.I. Murugachandran, M.E. Sanz	Spectrum assigned
C <sub>12</sub> H <sub>18</sub> O <sub>3</sub> ^	Hinoikitiol - ethanol	C. Medcraft, S.I. Murugachandran, M.E. Sanz	Spectrum assigned
C <sub>10</sub> H <sub>12</sub> O <sub>4</sub> S^	Hinoikitiol -SO <sub>2</sub>	C. Medcraft, S.I. Murugachandran, M.E. Sanz	Spectrum assigned
C <sub>10</sub> H <sub>16</sub> O <sub>2</sub> S^	Limonene -SO <sub>2</sub>	C. Medcraft, S.I. Murugachandran, M.E. Sanz	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>
$C_7H_8O_2$ ( $CH_3OC_6H_4OH$ )	Guaiacol	Timothy Zwier <sup>1</sup>	Experiments Completed: Assignments Completed including <sup>13</sup> C
$C_9H_9N$ ( $C_6H_5CH_2CH_2CN$ )	3-phenylpropionitrile	Timothy Zwier <sup>1</sup>	Experiments Completed: Assignments Completed
$C_8H_{10}O_3$ (( $CH_3O$ ) <sub>2</sub> $C_6H_4OH$ )	2,6-dimethoxyphenol	Timothy Zwier <sup>1</sup>	Experiments Completed
$C_9H_{10}O_2$ ( $CH_3OC_6H_4OHCHCH_2$ )	2-Methoxy-4-vinylphenol	Timothy Zwier <sup>1</sup> , Emilio Cocinero <sup>2</sup>	Experiments Completed: Assignments Completed
$C_4H_3O_2$ ( $OC_4H_3O$ )	2-furanyloxy radical	Timothy Zwier <sup>1</sup> , John Stanton <sup>3</sup>	Experiments Completed: Assignments Completed
$C_6H_5O_2$ ( $OC_6H_5O$ )	Hydroxyphenoxy radical	Timothy Zwier <sup>1</sup> , John Stanton <sup>3</sup>	Experiments Completed Preliminary Assignments
$C_6H_5O$	Phenoxy radical	Timothy Zwier <sup>1</sup> , John Stanton <sup>3</sup>	Experiments Completed Preliminary Assignments

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## IN MEMORIAM

### JAMES ROBERT DURIG



On January 7<sup>th</sup>, 2020, the field of molecular spectroscopy and molecular structure suffered the loss of one of its foremost practitioners: James R. (“Jim”) Durig. Jim was born in the Buffalo Township of western Pennsylvania on April 30<sup>th</sup>, 1935, and literally went to elementary school in a one-room schoolhouse. Jim’s interest in teaching was sparked in the fifth grade when the one (and only) teacher asked him to tutor a 16 year old 6<sup>th</sup> grader. He thought, “That sounds like it would be a good job, I’d probably like that.” This changed his life and he continued to tutor and teach through school, guided by the philosophy, “You learn by teaching.” Graduating from Claysville High School in 1953, Jim planned to become a high school history teacher, but was later informed that history teachers often worked as football coaches—at least in that part of the country—and that was not in his long-term plans.

Upon matriculating at Washington and Jefferson College, though, Jim was counseled that—given his aptitude in science—he should consider majoring in a science discipline instead of history. Eventually, he found Chemistry more interesting, and graduated from “W & J” *magna cum laude* with a B. A. degree in 1958, majoring in Chemistry and minoring in Mathematics. At W & J, Jim was elected to the Phi Beta Kappa honor society, the first of many significant honors to come. Deciding to pursue a graduate degree, Jim was awarded a Woodrow Wilson Fellowship at the Massachusetts Institute of Technology, where he earned a Ph.D. degree in Physical Chemistry with a minor in Physics.

At MIT, Jim opted to undertake research in molecular spectroscopy under the supervision of Professor Richard Collins Lord. Upon joining the Lord lab, Jim

soon became a mentee of a more senior graduate student in the Spectroscopy Lab, Walter J. (“Walt”) Lafferty. In fact, on Jim’s first scientific publication, on the far infrared spectrum of disiloxane, Walt was one of the co-authors. [After Walt graduated from MIT in 1961, and conducted post-doctoral research at Johns Hopkins University, he secured a position at the National Bureau of Standards (now the National Institute of Standards and Technology), where, in 1968, Jim would later undertake a sabbatical leave, and they would be co-authors on two more scientific publications.]

After graduating from MIT in 1962, Jim obtained a faculty appointment at the University of South Carolina (USC) as an Assistant Professor in the Department of Chemistry. He quickly rose through the academic ranks, and in 1970 was appointed to a named professorship—as an Educational Foundation Professor of Chemistry. Three years later, Jim undertook the Deanship of the College of Science and Mathematics, a title he held for 20 years, before becoming the Dean of the College of Arts and Sciences at the University of Missouri-Kansas City (UMKC) in 1993. Then in 2003, Jim was subsequently appointed to the highest academic rank in the University of Missouri system: that of Curators’ Professor (of Chemistry and Geosciences in his case). In 2016, Jim retired from UMKC as a Curators’ Professor Emeritus.

At South Carolina, Jim launched his career as an independent scientist by acquiring infrared, Raman and far infrared instrumentation with funding from university, state and federal sources (NSF), and he recruited graduate students to help pursue his interests in vibrational spectroscopy and molecular structure of small molecules. Some of the early projects carried out included compounds containing second period heteroatoms like boron and nitrogen, as well as heavier elements such as phosphorus, silicon, sulfur, germanium, tin, bromine or iodine, and even some transition metal complexes of palladium and ruthenium. Studies of low frequency, large amplitude vibrations such as ring puckerings and bendings, as well as torsional oscillations soon followed—as did conformational analysis.

In 1968, though, Jim spent a sabbatical leave at the National Bureau of Standards, where he teamed up again with Walt Lafferty, and initiated his research pursuits in microwave rotational spectroscopy. Jim was successful in obtaining funding from the National Science Foundation to acquire a microwave instrument

(the Hewlett- Packard 8640A MRR spectrometer), which incorporated a backward wave oscillator source and 33.3 kHz Stark modulation, covering the 12.4 to 40.0 GHz frequency range. This instrument was installed at USC and began operating by late 1970 and early 1971. Along with the new microwave spectrometer, Jim hired a post-doc (Y. S. Li) with substantial microwave experience. Dr. Li had obtained his Ph.D. with Marlin Harmony at the University of Kansas and was a post-doc with Victor Laurie at Princeton. Jim's graduate students were encouraged to expand their molecular spectroscopic expertise to include pure rotational spectroscopy in addition to vibrational spectroscopy. The first publication from the Durig lab that incorporated microwave results (on the microwave spectrum of 2,3-dihydrofuran), was submitted in August of 1971 and appeared in the *Journal of Chemical Physics* in June of 1972 (Volume 56, page 5682). In fact, a total of eight articles from the Durig lab that involved microwave spectra appeared in print in 1972, ten in 1973 and twelve in 1974. An impressive number of further publications involving microwave spectroscopy followed in rapid succession over the next 40+ years.

And while the Hewlett Packard instrument accompanied Jim to UMKC in 1993, it was already showing signs of aging, and was never fully operational again. Nevertheless, Jim and his students were still able to obtain microwave spectra through collaborative efforts and instrument time with such microwave spectroscopists as Brooks Pate at the University of Virginia, Sean and Rebecca Peebles (Eastern Illinois University), or Michael Tubergen at Kent State University. When Garry Grubbs took a position at the Missouri University of Science and Technology (in Rolla), Jim explored the possibility of collaborating within the University of Missouri System, but that potential joining of forces was ultimately suspended when Jim retired in 2016.

Jim's rotational spectroscopy publications spanned the range of molecular information that microwave spectroscopy is capable of providing. This included, among other results: rotational constants, centrifugal distortion constants, either complete or nearly complete  $r_0$  and  $r_s$  structures, molecular conformations, low-frequency vibrational data from excited states (complementing Jim's vibrational studies), nuclear quadrupole coupling constants in molecules containing one or two N, Cl, Br and I atoms, and internal rotation involving one or two rotors and their associated potential energy functions. Once computational chemical software

became more generally available, Jim's research group began incorporating *ab initio* and density functional theory calculations into its repertoire of methods for establishing detailed molecular structures, and even developed a program ("A and M," for *ab initio* and microwave) for arriving at structural parameters by essentially combining information from both approaches.

Jim Durig's lifelong research interests all involved determining what is perhaps the most basic information about a chemical substance—namely its molecular structure. In obtaining those molecular structures, Jim initially focused on using vibrational spectroscopy, ranging from the mid-infrared region to the far-infrared region for photon absorption, as well as Raman spectra for scattering of the photons. He and his research group carried those experiments out in the gaseous, liquid, and solid states, and in solution as well (using solutions in liquefied noble gases more recently), and variable temperature studies were also performed to help determine the energetics involved in conformational equilibria. Subsequently, the Durig group was able to incorporate microwave rotational spectroscopy and computational chemistry methods successfully in establishing gas phase molecular structures. It is not surprising then, given his longstanding interest in molecular structure, that Jim was also a co-author on seven collaborative publications using electron diffraction methodologies.

In investigating molecular structures, Jim Durig was extraordinarily successful and productive. Perhaps it is apocryphal, but Jim claimed that when he interviewed at the University of South Carolina in 1962, he was asked by the then-Dean about what his professional goals as a faculty member would be. In answering that question, Jim purportedly stated, "publish 1,000 research papers, and graduate 100 Ph.D. students." In typical Jim Durig fashion, he exceeded both of those goals (with 1079 publications and 120 Ph.D. graduates). Along the way, he collaborated with scientists across the globe too numerous to cite here, and earned many, many awards and honors. Primary among those honors were ones which were more specifically related to spectroscopy, such as: the Coblentz Society Award; the Spectroscopy Society of Pittsburgh Award; the Southern Chemist Award; the Alexander von Humboldt Senior Scientist Award; and the Sir Harold Thompson Memorial Award, "for significant accomplishments to spectroscopy reported in *Spectrochimica Acta*."

Finally, we would be remiss in failing to mention that Jim Durig was far more than simply a world-class researcher. He was a fine teacher, a longtime and especially effective academic administrator (Dean at South Carolina for 20 years and 7 years at UMKC), Editor or Editorial Board member of five spectroscopic journals, Editor of nearly thirty books (including the more than two dozen volume series, *Vibrational Spectra and Structure*), and Fellow of several professional scientific societies. He also organized and Chaired a half-dozen or so international scientific conferences in Raman spectroscopy, Fourier transform infrared spectroscopy, and low temperature chemistry, along with two NATO Advanced Study Institutes on spectroscopic topics.

Both within and beyond the university, Jim Durig actively encouraged and involved students at all levels in the pursuit of scientific discovery and knowledge attainment. Equally worth noting, if not more importantly perhaps, was Jim's steadfast promotion of under-represented groups—women and minorities—in the STEM disciplines. Furthermore, since numerous researchers from across the globe sought out and visited Jim's "spec labs" in South Carolina and Missouri over the years, students, post-docs and colleagues of Jim were provided unique opportunities to learn more—not only about science, but also other cultures.

From the forgoing discussion then, it should be clear that Jim Durig accomplished a huge amount in his nearly 85 years of time on Earth. Somehow, he was able to extract more than 24 hours out of each day. Of course, he could not have accomplished as much as he did without the unwavering support of his wife, Marlene, and his family: sons Douglas and Bryan, and daughter Stacey.

While he has left us, though, Jim's legacy will live on through all of those he taught, supervised or interacted with, and we—along with the entire molecular spectroscopic community—mourn his passing.

Peter Groner  
Victor F. Kalasinsky  
Y. S. Li  
Charles J. Wurrey

Postscript: For those who would be interested, please see the excellent overview of molecular spectroscopy research at the University of South Carolina, written as an Editorial by Jim Durig himself in 1993 for a special issue of *Spectrochimica Acta*, **49A**, pages 1827-1832.

Obituary – Provided by Gamil Guirgis



Dr. James Robert Durig COLUMBIA Dr. James Robert Durig, 84, passed away on Tuesday, January 7, 2020. Funeral services will be held 11:00 am Saturday, January 11, 2020 at Dunbar Funeral Home, Devine Street Chapel with burial to follow at Elmwood Cemetery. A gathering of family and friends will be one

hour prior to the service at the funeral home and immediately following the graveside service in the chapel at Elmwood Cemetery. Dr. Durig was born April 30, 1935 in the Buffalo Township of Washington County, Pennsylvania. He graduated from Claysville High School in 1953. After working with the B&O Railroad for a year, he entered Washington and Jefferson College. He graduated in 1958, Magna Cum Laude and was elected to Phi Beta Kappa. He was awarded the Woodrow Wilson Fellowship to earn his doctorate in physical chemistry at the Massachusetts Institute of Technology. He is a Distinguished Professor Emeritus at the University of South Carolina where he was a professor from 1962 to 1993 and Dean of the College of Science and Mathematics from 1973 to 1993. He is an Emeritus Professor at the University of Missouri-Kansas City where he was Dean of the College of Arts and Sciences from 1993-2000 and a professor from 1993-2016. Dr. Durig was one of the most distinguished chemists in the global scientific community. In his 48 years of teaching, he has supervised more than 100 doctoral students and authored over 1,000 academic refereed journal articles about vibrational and rotational spectroscopy. Dr. Durig also participated in conferences and gave lectures on his scientific expertise all over the world. He is predeceased by his mother, Roberta Durig; his wife of 60 years, Marlene Sprowls Durig; and brother Bruce Mounts. Survivors include his brothers, Melvin Mounts of Green Valley, AZ and Earl Mounts of Pittsburgh, PA; his children, Douglas Durig of Sewanee, TN, Bryan Durig (Marla) of Columbia and Stacey Hamm (Kurt) of Columbia; and grandchildren, Nicole Durig Quinlan (Rick), Mallory Durig, Delaney Durig, Meagan Durig, Kathryn Hamm, Jamie Hamm, and Laura Hamm. In lieu of flowers, memorial contributions may be made to the Alzheimer's Foundation; or to the [charity of one's choice](#). Please sign the online guestbook at [www.dunbarfunerals.com](http://www.dunbarfunerals.com). Memories may be shared at [www.dunbarfunerals.com](http://www.dunbarfunerals.com)



## IN MEMORIAM

### Harald Møllendal



Our good friend and colleague Harald Møllendal passed away on July 13 after a short illness at 75 years old. He was born and had a happy childhood in Ålesund. After graduating from high school, he did his military service, and studied science at the University of Oslo (UiO). After graduate studies and a postdoctoral period abroad, he obtained his doctorate, and from 1976 he was associate professor, later professor, in physical chemistry at the Department of Chemistry, UiO.

Throughout his career, Harald used physical and mathematical methods in his research. His research included measuring and describing the structure, conformation and internal interactions of molecules, hydrogen bonds, which are of fundamental importance for understanding proteins and enzyme activity. He was an internationally recognized expert in this field. In later years, astrochemistry became a central theme for him. The weak microwave radiation from molecules in the almost empty space between the stars makes it possible to identify chemical compounds light years away from Earth. He, together with colleagues at home and abroad, has published more than 200 academic papers. In 2010 he received the Mez-Starck Prize for "outstanding contributions in the field of structural chemistry and high resolution molecular spectroscopy".

At the Department of Chemistry, Harald was known as a very capable teacher, populizer of science and supervisor. In addition, he held a number of administrative positions at UiO.

Harald Møllendal was particularly well liked by his colleagues who he selflessly helped in large and small. It is a pity that an acute illness so brutally put an end to such a considerable scientific career. We send a warm greeting to his wife for 50 years, Wenche, and their three children.

On behalf of his colleagues, in deep respect,  
Peter Kleebe  
Svein Samdal  
Einar Uggerud