

**NRC-CNRC**

*Steacie Institute  
for Molecular  
Sciences*

# Canadian Program (?) (Lab Spectroscopy)

**A.R.W. McKellar**

**Steacie Institute for Molecular Sciences  
National Research Council of Canada**



National Research  
Council Canada

Conseil national  
de recherches Canada

Canada 

# *Canadian Spectroscopy, coast to coast*

**Walter Balfour**, University of Victoria

- electronic spectroscopy

**Merer, Ozier, Signorell, Hepburn, Momose**, University of British Columbia

- spectroscopy

**Mike Gerry**, University of British Columbia

- microwave spectroscopy

**Wolfgang Jäger**, University of Alberta

- microwave, mm-wave, ir spectroscopy

**Yunjie Xu**, University of Alberta

- ir, microwave spectroscopy

**Nasser Moazzen-Ahmadi**, University of Calgary

- ir spectroscopy

**Yujun Shi**, University of Calgary

- electronic spectroscopy

**Adriana Predoi-Cross**, University of Lethbridge

- ir spectroscopy, atmospheric physics

**Dominique Appadoo**, University of Saskatchewan

- ir spectroscopy

**Jennifer van Wijngaarten**, University of Manitoba

- microwave spectroscopy

**T. Reddish, B. Atkinson, L. Krause**, University of Windsor

- electronic spectroscopy

# *Canadian Spectroscopy, coast to coast*

**Rob Lipson**, University of Western Ontario

- electronic spectroscopy

**Peter Bernath**, University of Waterloo

- spectroscopy

**Takayoshi Amano**, University of Waterloo

- mm-wave spectroscopy

**Kaley Walker**, University of Toronto

- microwave spectroscopy, atmospheric physics

**Bob McKellar**, National Research Council

- ir spectroscopy

**Klaus Huber, Benoit Simard**, National Research Council

- electronic spectroscopy

**Hans-Peter Loock**, Queen's University

- electronic spectroscopy

**Li-Hong Xu, Ron Lees**, University of New Brunswick

- ir, microwave spectroscopy

**Dennis Tokaryk**, University of New Brunswick

- spectroscopy

**Colan Linton, Alan Adam**, University of New Brunswick

- electronic spectroscopy

**John Coxon**, Dalhousie University

- electronic spectroscopy

# ***Canadian Spectroscopy, coast to coast***

**Wolfgang Jäger, University of Alberta**

- microwave, mm-wave, IR spectroscopy; weakly-bound complexes and clusters, helium droplets

**Yunjie Xu, University of Alberta**

- IR, microwave spectroscopy; interactions of chiral molecules

**Nasser Moazzen-Ahmadi, University of Calgary**

- IR spectroscopy; internal rotation, carbon chains & other unstable species

**Adriana Predoi-Cross, University of Lethbridge**

- IR spectroscopy; atmospheric applications: line broadening & mixing, intensities, remote sensing

**Dominique Appadoo, University of Saskatchewan**

- far-IR synchrotron spectroscopy

**Jennifer van Wijngaarten, University of Manitoba**

- FTMW spectroscopy of molecular ions; far synchrotron spectroscopy

# *Canadian Spectroscopy, coast to coast*

**Peter Bernath**, University of Waterloo

- spectroscopy, radicals & ions, hot molecules

**Takayoshi Amano**, University of Waterloo

- mm-wave spectroscopy, radicals & ions

**Kaley Walker**, University of Toronto

- FTMW spectroscopy (atmospheric molecules, e.g. CClBr), atmospheric physics, remote sensing

**Bob McKellar**, National Research Council

- IR spectroscopy; far-IR synchrotron spectroscopy, weakly-bound complexes and clusters; mm-wave

**Li-Hong Xu, Ron Lees**, University of New Brunswick

- IR, microwave spectroscopy; methanol; internal rotation

**Dennis Tokaryk**, University of New Brunswick

- spectroscopy; far-IR synchrotron spectroscopy; radicals & ions

# *Can synchrotron IR contribute ?*

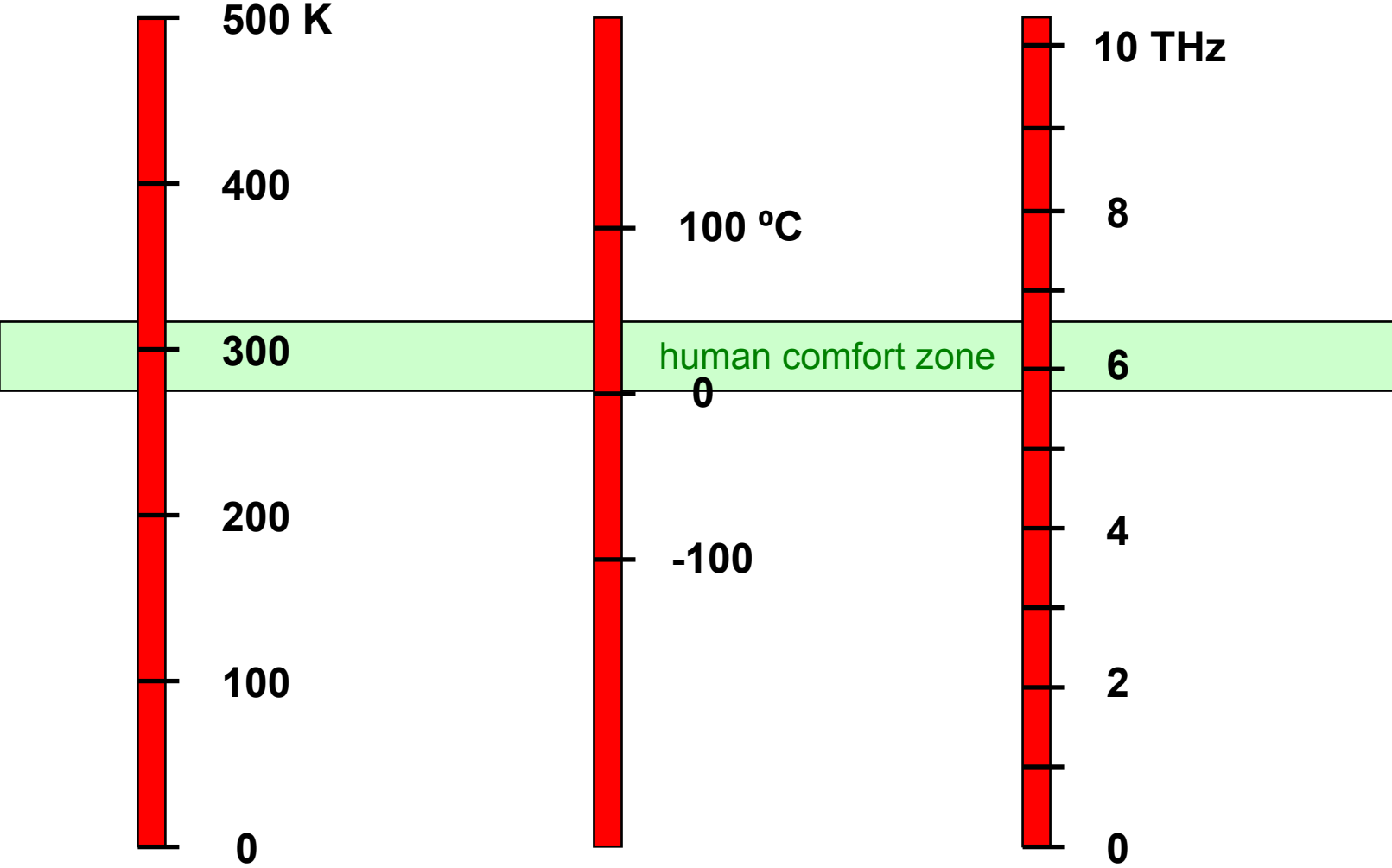


**We have a far infrared beamline for high resolution gas-phase spectroscopy at the Canadian Light Source in Saskatoon**

*Kelvin  
thermometer*

*Celsius  
thermometer*

*Terahertz  
thermometer*



# Where is Saskatoon?





# *Background*

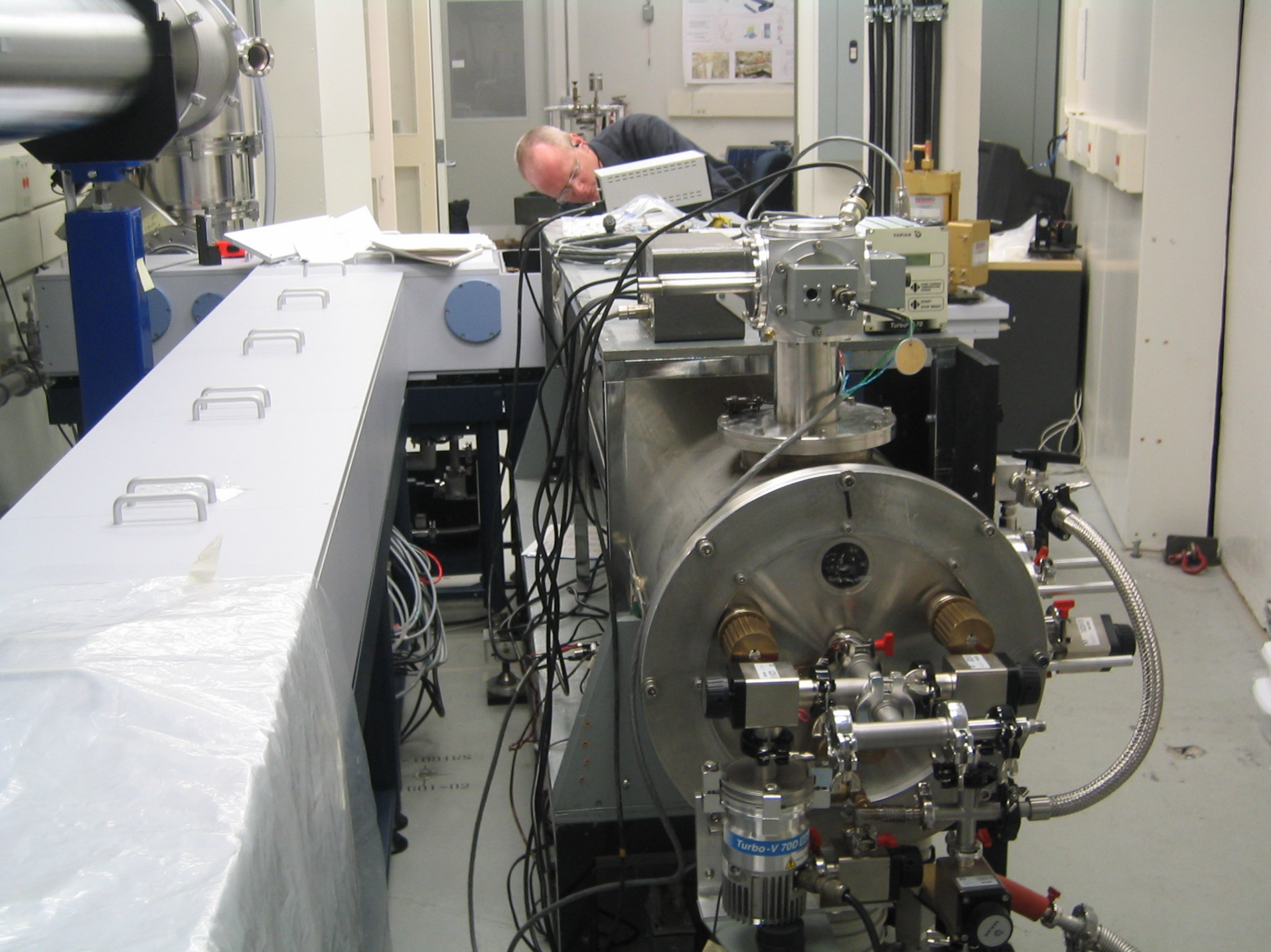
synchrotron infrared



**The synchrotron simply replaces the normal thermal source (globar), providing continuum IR radiation to a conventional (high quality) FTIR spectrometer**

**The high brightness of synchrotron radiation is ideal for the small entrance aperture required for high spectral resolution**

**Our Bruker IFS 125 HR spectrometer has a maximum optical path difference of 9.4 m, giving an instrumental resolution of  $\sim 0.0008 \text{ cm}^{-1}$  (24 MHz)**



# *Previous hi-res synchrotron IR*

**Noise is the big problem!**

**Results from MAXlab and LURE were promising, but did not fully achieve the synchrotron advantage**

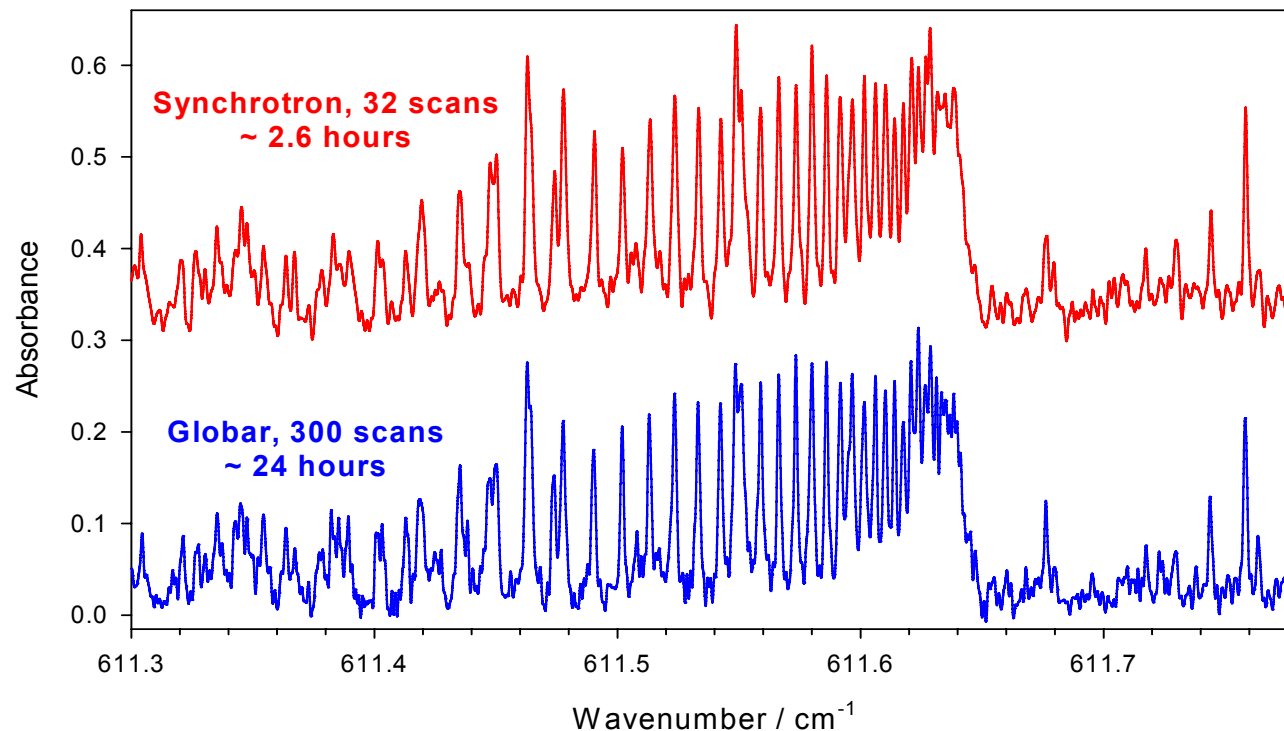
**We hope to do significantly better**

**SOLEIL, Australia, Switzerland, ... are also planning new gas-phase IR facilities**

**Will we be the first synchrotron user facility for high-res IR spectroscopy of gases?**

# First far-IR results from CLS

$\nu_{17}$  band  
of acrolein  
( $\text{CH}_2\text{CHCHO}$ ,  
propenal)



**The beamline is now in the commissioning phase**

**We are doing well around  $600 \text{ cm}^{-1}$ , but there is a lot of noise below  $\sim 200 \text{ cm}^{-1}$**

# ***Synchrotron/FTS vs. 'real' THz spectroscopy***

**The resolution (and sensitivity?) of the synchrotron/FTS combination is clearly inferior to that of 'real' mm-wave spectroscopy. And the optimum frequency range (i.e.  $> 1.7$  THz) is too high for direct observation of many rotational transitions of interest**

**But there is a big advantage: *massively parallel data acquisition***

**Tens of thousands of transitions are measured simultaneously, which could be advantageous for some astrophysical data needs!**

**Compared to a conventional source, the synchrotron brightness allows a high resolution spectrum to be recorded in much shorter time (say, 1 hr vs. 30 hr)**

# A Targeted Canadian Project ?

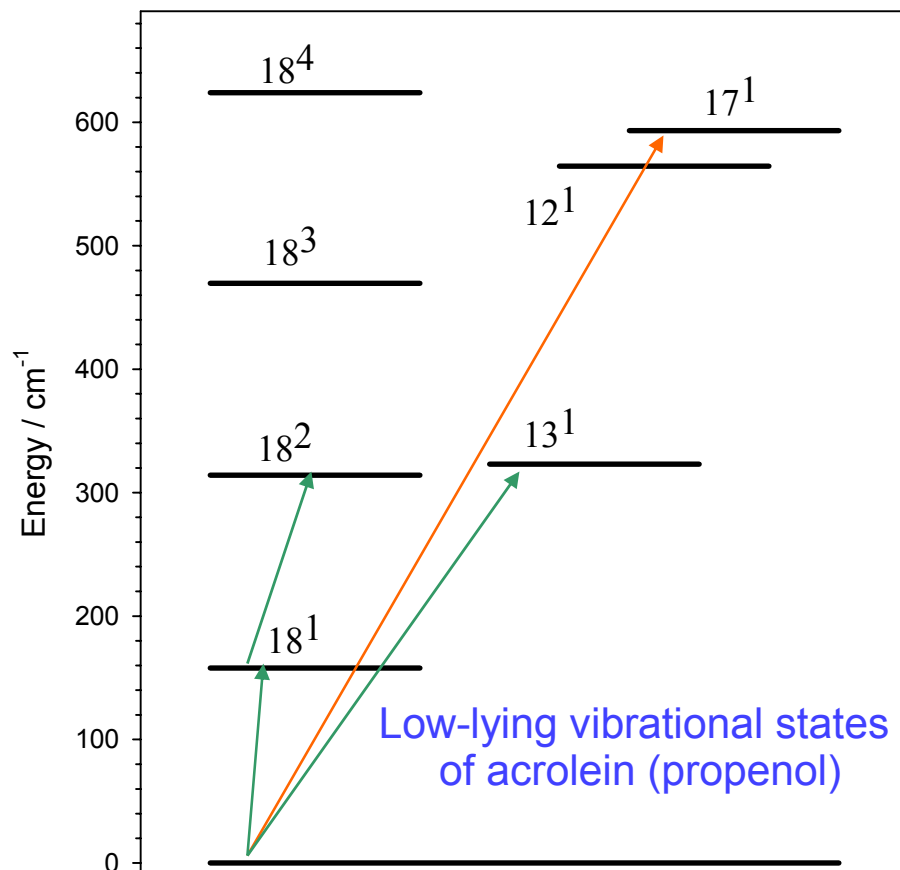
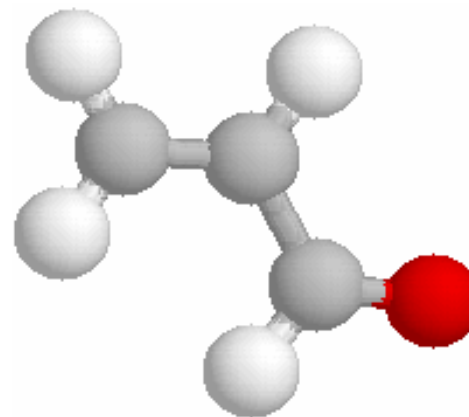
The **Special Research Opportunity** (SRO) program supports unique, emerging research opportunities that are timely, urgent, high-risk or have a strong potential for breakthrough that will be of substantial benefit to Canada. The program also supports pre-research activities to investigate and develop potential new collaborative projects necessary to respond to these national and international opportunities.



## ***Projects that may be considered by the SRO program:***

- **A project that can be undertaken only in conjunction with a specific and unusual world event**
- **A workshop to define and plan Canadian participation in a major international research initiative**
- **An interdisciplinary effort to address an emerging problem of importance to Canada**
- **A project that leads to, or exploits, a breakthrough discovery which establishes or maintains Canada's international leadership position in a niche area**
- **A novel, high risk project with the potential to change the direction of thought in a discipline or open up new areas of discovery**
- **The special opportunity must be unique, unforeseen, and outside the normal evolution and advancement of a longer term research program. It is timely and linked to a window of opportunity that did not exist a year ago, and will not exist in the future.**
- **In addition, the research project must be novel, high risk, or have a strong potential for breakthrough.**
- **Advancements of ongoing research and collaboration, such as research supported through an NSERC Discovery Grant, do not constitute a special opportunity.**

# Acrolein

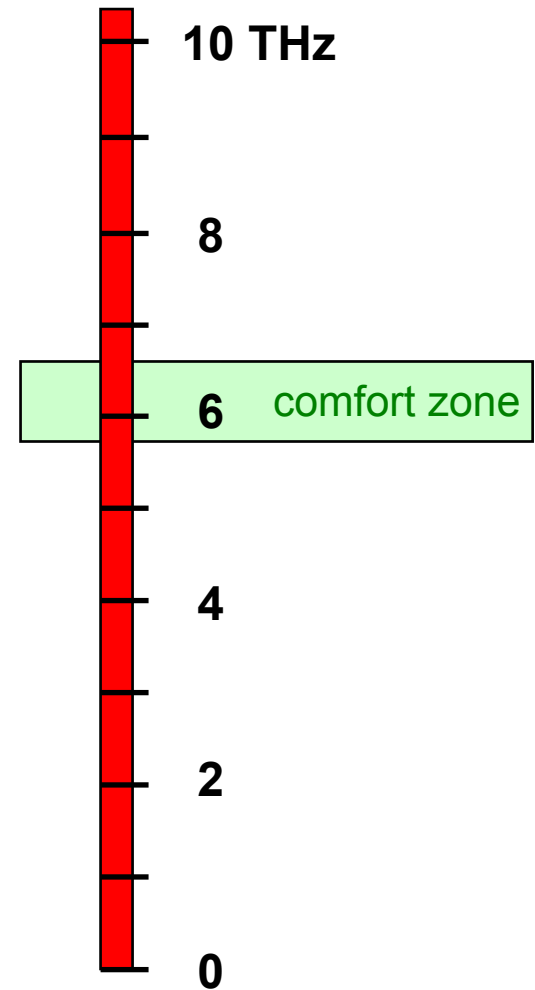


	<b>18<sup>1</sup></b>	ground state
$\nu_0$	<b>157.8834</b>	
<b>A</b>	<b>1.54267</b>	1.57955
<b>B</b>	<b>0.15565</b>	0.15542
<b>C</b>	<b>0.14209</b>	0.14152

# ***THz Astrophysics***

*Do extraterrestrials  
also prefer the 6 THz  
comfort zone?*

*Terahertz  
thermometer*





## *Terahertz thermometer*

