

White Paper ID Number	W056
Title of White Paper	Molecular Astrophysics \& Astrochemistry
ID of Associated Expression of Interest	E063
Topic Area of White Paper	<div style="background-color: #e6f2ff; padding: 5px; border: 1px solid #c0d9ff;">science programs, science topics and science themes</div> <div style="background-color: #e6f2ff; padding: 5px; border: 1px solid #c0d9ff; margin-top: 5px;">laboratory astrophysics</div>

Executive Summary of White Paper (5000 character limit)

Many of the facilities and missions that Canada is or will be involved in as well as the diverse science programs that drive these missions rely on the astronomical detection and characterization of atomic and molecular gas as well as dust grains across the electromagnetic spectrum. Molecular bands and dust features have been observed in almost all astrophysical environments – from exoplanet atmospheres to interstellar clouds and star forming regions to AGN winds. Indeed, to date, over 200 molecules and a handful of minerals have been identified in space, and the Universe is aglow with the widespread and abundant emission of Polycyclic Aromatic Hydrocarbons (PAHs). Molecules and dust grains can be powerful probes for the physical conditions in the environment in which they reside, and their presence can help elucidate chemical evolution. However, the vast majority of the known molecular spectral features remain unidentified, and for many identified species, we do not have enough information to turn their spectral appearance into diagnostic probes. Support from laboratory experiments, theoretical calculations and detailed observational data analysis will be crucial to fully exploit astronomical observations in the next decade. This white paper describes the current expertise in Canada in the fields of molecular astrophysics and astrochemistry, detail the key science questions to address within the next decade, and describe the expected needs from laboratory astrophysics and computational chemistry to establish a unique Canadian expertise center in molecular astrophysics and astrochemistry to support upcoming astronomical missions and facilities.

Lead author and affiliation	Jan Cami, Western University
Email address of lead author	jcami@uwo.ca

Other authors and affiliations

Els Peeters & Martin House, Western University
Margot Mandy, The University of Northern British Columbia
Rene Plume, University of Calgary
Doug Johnstone, NRC-Herzberg
Nienke van der Marel, NRC-Herzberg
Sarah Sadavoy, Queen's University
Alex Hill, UBC

Molecular Astrophysics & Astrochemistry

1 Canada's Place in The Molecular Universe

Astronomical observations across the electromagnetic spectrum often carry the imprint of molecular species and dust grains. To date, about 200 individual molecular species have been identified in space¹ and many hundreds more await identification. The molecules we have been able to identify show a wide range in sizes, structures, shapes and chemical compositions – ranging from small and simple diatomics such as H₂ and CO to more complex organics and large aromatic molecules like C₆₀ and C₇₀. We have found these molecules in meteorites, comets, planets and other Solar System bodies (Ehrenfreund & Charnley, 2000). Even the harsh environment of the diffuse interstellar medium (ISM) harbours a surprisingly rich molecular inventory, as do molecular clouds, star-forming regions, proto-planetary disks, exoplanet atmospheres and the surroundings of dying stars. On larger scales, we have clearly seen the fingerprints of molecular species (and in particular of polycyclic aromatic hydrocarbons, PAHs) in massive starburst galaxies and in the active galactic nuclei of distant galaxies, out to $z \sim 6$ (Riechers et al., 2014). We have learned that the molecular inventory is not static, but is shaped by the governing processes and available materials in different environments. Molecules form in the outflows of evolved stars; this material is then processed in the ISM by UV radiation, energetic particles and shocks after which they end up in newly formed stars and planets. The chemical pathways involve bottom-up reactions whereby atoms and molecules combine to form larger species, but in recent years, it has become clear that also top-down processes are important in which larger molecules and dust grains are broken up into smaller molecules. Note that molecular formation, growth and destruction needs to be considered in the gas phase as well as on ice mantles (Boogert et al., 2015) and the surfaces of dust grains. The result is a rich variety in molecular species. In turn, these molecules are themselves responsible for key physical processes that directly affect their environment. In dense molecular clouds for instance, they dominate gas cooling and control the ionization balance and this then affects how the magnetic field couples to the gas. In the ISM on the other hand, large molecules are major contributors to the heating (through the photo-electric effect). This way, molecules drive much of the large-scale processes in the Universe, including star and planet formation, and the evolution of galaxies (Tielens, 2013). Many of these molecular species furthermore contain the carbon that ultimately finds its way into biologically relevant molecules; these building blocks of life are thus seeded throughout the cosmos. In addition to their scientific relevance, molecules hold an enormous diagnostic power. The precise details of molecular spectral features can encode a wealth of information about the physical and chemical environment in which they reside. Molecules are thus ideally suited to study many astrophysical processes in the Universe quantitatively. In summary, it has become clear that we truly live in a *Molecular Universe*: the Universe is rich in a bewildering variety of molecules that are widespread and abundant throughout the Universe; they are found in many different astronomical environments where they play key roles in large-scale astrophysical processes; they include prebiotic interstellar molecules that may represent the first steps toward life; and they can be used to trace important processes and provide information about their environment (Tielens, 2013).

Canada has a rich heritage in molecular spectroscopy through the likes of Nobel laureate Gerhard Herzberg – a chemist who made an enormous contribution to astronomy. This heritage furthermore shows in the sizeable fraction of the Canadian astronomical facilities that are ideally suited to (if not designed for) detect and characterize molecular spectral signatures – from the spectrographs on the CFHT to participation in facilities such as Gemini, ALMA, JWST and possibly future missions such as SPICA. Not surprisingly then, there is a fair deal of astronomy research in Canada that employs these facilities and hence uses molecular spectroscopy as an important diagnostic tool. Canada is however also an internationally respected contributor to research on molecular astrophysics and astrochemistry – the research fields that study the physical processes that molecules undergo in astronomical environments and the chemistry that is the result of it. Note that the two terms are often used interchangeably, and that the nucleation and processing of dust can be included as well. Thus, there is a direct connection to several other white papers, and in particular to W005: Signposts of planet formation in protoplanetary disks, van der Marel et

¹see <https://zeus.ph1.uni-koeln.de/cdms/molecules>

al.; W017: Star Formation in the Galactic Ecosystem, Rosolowsky et al.; W029: The Life Cycle of Dust, Sadavoy et al.; W035: Mid- Through Far-Infrared Astronomy: The Path to Tomorrow, Johnstone et al.; W044: Canadian Investigations of the Interstellar Medium, Hill et al.; W048: Science with ground based single-dish submillimeter wave telescopes, Chapman et al.; W049: SPICA: The next observatory class infrared space astronomy mission, Naylor et al.; E038: Entering a New Era of Astrophysics with the James Webb Space Telescope, Doyon et al.; E025: The Formation of Stars - From Filaments and Cores to Protostars and Protoplanetary Systems, di Francesco et al.

2 Scientific opportunities in an interdisciplinary field

Many astronomers are familiar with tools that employ molecular spectral features as diagnostic tools for astrophysical processes, such as e.g. rotation diagrams or tools that use emission of polycyclic aromatic hydrocarbon (PAH) molecules to determine star formation rates (see e.g. Maragkoudakis et al., 2018). There is often much “under the hood” work that is required to create such tools: identifying what molecular species or dust mineral causes what spectral features; establishing how molecules in space respond to changes in their environment and what the resulting chemistry is; working out the details of the physical processes happening at the molecular scale (at conditions relevant to astronomical environments!); calculating or experimentally measuring all relevant rates; and finally creating a complete model that is based on a fundamental and quantitative understanding of all this molecular astrophysics and astrochemistry and that can be used to create the tools that astronomers require.

Many of these steps require a close interaction and collaboration between researchers in different fields: observational and theoretical astronomers, experimental and computational chemists, molecular physicists, computer scientists, material scientists and mineralogists. Molecular astrophysics and astrochemistry are thus highly interdisciplinary fields. Canadian astronomers have contributed to various aspects of this enterprise, and are in a good position to make significant progress in the field in the next decade. Such progress is particularly desirable, since it increases the scientific return of many Canadian facilities and research areas.

2.1 Large molecules, nanoparticles and dust in the interstellar medium

A sizeable fraction of the cosmic carbon ($\sim 15\%$) is in the form of a population of large molecules that are widespread and abundant in the Universe, and that reveal themselves through literally hundreds of spectral feature from the near-UV to the mid-IR (and likely also at longer wavelengths) that furthermore show significant sightline-to-sightline variations. It is clear that these molecules harbour an enormous potential as diagnostic tools, but there are several hurdles to clear before those will materialize.

Infrared observations since the 70s have indeed revealed strong and widespread emission features in the Universe near and far that are commonly ascribed to vibrational motions of PAHs and closely related species (Tielens, 2008; Peeters, 2014). However, since these features are common to almost all such molecules, not a single PAH species has been reliably identified to date, and hence it is not clear what the properties are of the underlying PAH population. This has greatly hampered the development of a complete description for such species in space and consequently also the development of accurate quantitative tools. Much progress can be expected from mid-IR observations with the JWST, and Canadian astronomers lead a successful ERS program that will provide an unprecedented, detailed look at how the PAH emission characteristics change as one moves through a photo-dissociation region from the molecular cloud to the ionized region. Key is the close collaboration between astronomers and the experimental and theoretical chemists that have produced the NASA Ames PAH Database.

The only currently identified large molecules in space are a few different flavours of fullerenes: neutral C_{60} and C_{70} (Cami et al., 2010) and C_{60}^+ (Campbell et al., 2015). Especially C_{60} is found to be widespread and abundant in our Milky Way and other galaxies as well (Cami, 2015). But while the presence of fullerenes in space was expected since they were first discovered on Earth (Kroto et al., 1985), the astronomical observations have revealed big gaps in our understanding of the chemistry of large molecules as well as in the molecular processes that govern their excitation. Indeed, we currently do not know what the formation routes are towards fullerenes (Cami et al., 2018), and our quantitative models to explain the absorption of C_{60}^+ as well as those to explain the IR emission of C_{60} fall

short of reproducing the available observations. One clear finding that resulted from studies on cosmic fullerenes is the importance of UV photo-processing and the resulting top-down chemistry. While originally investigated as a possible route to C_{60} from large PAHs (Berné & Tielens, 2012; Zhen et al., 2014), the process is of course much more general and will significantly affect the chemistry in the ISM. Since many of the molecular properties of fullerenes are very similar to those of PAHs, any progress in understanding the fundamental details of fullerenes in space will have an enormous impact on our understanding of PAHs in space as well. Here too, observations with the JWST will greatly advance our understanding by mapping out how the emission bands change as a function of physical parameters.

A closely related problem is that of the diffuse interstellar bands (DIBs), a set of about 600 interstellar absorption bands from the near-UV to the near-IR that are routinely observed in reddened stars (see e.g. the compilation of DIB research in Cami & Cox 2014 and the recent survey by Fan et al. 2019). Their interstellar nature is well established, but with one exception, the species that cause these features remain unidentified. Given that the first DIBs were observed in 1919 (Heger, 1922), this represents the longest standing problem in astronomical spectroscopy. Only a few years ago, the first few DIBs in the near-IR were reliably identified as due to C_{60}^+ (Campbell et al., 2015; Walker et al., 2017; Cordiner et al., 2019). The remaining DIB carriers are thought to be stable and abundant carbonaceous molecules such as PAHs, other fullerene compounds or carbon chains. Ultimately, an identification requires a good match with a proper laboratory spectrum. However, the sheer number of possible molecules to consider, and the many experimental challenges involved in obtaining spectra of such molecules under conditions that are comparable to those in space make this a daunting enterprise. Much guidance to laboratory astrophysics is expected from current observational studies (see e.g. Cox et al., 2017) that are placing strong constraints on the properties of the carrier molecules from detailed observational analyses of the DIBs. Studies of the variations in the DIB line profiles coupled with state-of-the-art electronic structure calculations and ro-vibrational contour modeling can greatly help to elucidate some of the physical processes that occur.

In addition, there is presently an ongoing debate about the role of dust in astrochemistry, and this based on two different lines of thought. First, the dust destruction rate in the ISM is higher than the formation rate by evolved stars, and thus some form of replenishment is required (Tielens, 2005). Laboratory experiments have recently hinted at the possibility of barrierless reactions on the surfaces of dust grains (Fulvio et al., 2017; Krasnokutski et al., 2017). If such reactions are common, it could explain how dust can be created and grown in the ISM itself. At the same time, it has become clear that especially in radiative environments, photo-processing induces a top-down chemistry that has been overlooked for many decades (Zhen et al., 2014). It is not clear at this point how viable this photo-processing is in the ISM, or which of the photoproducts could be stable in such environments, but such processes could play important roles in explaining the chemistry in the ISM (see also the WPs by Sadavoy et al. and Johnstone et al.).

2.2 Molecular line polarisation to probe magnetic fields in star-forming regions and circumstellar disks

For several decades astronomers have used measurements of linear polarisation from dust to study the morphology and (indirectly) the strength of magnetic fields in star-forming regions. Given the successes obtained with this technique it was logical to expect that its application to much higher spatial resolutions with ALMA would allow us to reveal the structure and role of the magnetic field in the evolution of circumstellar disks and, ultimately, in the formation of planetary systems. Although recent dust polarisation studies using ALMA are indeed helping to characterize magnetic fields in protostellar systems (see for example Maury et al., 2018), it has become clear that at the highest spatial resolutions dust polarization does not consistently trace the orientation of magnetic field lines. This is due to the fact that, for example, radiation from the larger dust grains present in circumstellar disks tend to self-scatter and produce linear polarisation patterns that have little to do with the orientation of the ambient magnetic field (Kataoka et al., 2016).

As a result of this discovery astronomers have naturally turned to measurements of linear polarisation from molecular lines, which are free from this self-scattering process. The existence of molecular linear polarisation, believed to stem from the so-called Goldreich-Kylafis effect (Goldreich & Kylafis, 1981), has been verified obser-

tionally more than 20 years ago and has since been used for studying magnetic fields. There are, however, a couple of issues that stand in the way of the large-scale application of this technique:

1. The theoretical prediction and modelling of linear polarization levels have been worked out only for simple molecules such as CO (Cortes et al., 2005). The successful interpretation of observations from more complicated molecules observed in circumstellar disks will require the development of models for more complicated molecules.
2. It has also become clear in recent years, both on theoretical and observational grounds, that molecular transitions from species weakly sensitive to the Zeeman effect (such as CO and other molecules used for linear polarisation studies) also show circular polarisation signals in their spectra (Houde et al., 2013). These signals arise from the conversion of linear to circular polarisation as the detected radiation travels from background through foreground regions. More importantly, this conversion process brings a rotation in the orientation of the linear polarisation, and therefore masks its correlation to the morphology of the magnetic field. Once again the modelling of circular polarisation signals has been worked out for simple linear molecules (e.g., CO, HCN and SiO) but more work is needed to effectively use more complicated molecules for magnetic field studies and recovering its morphology from the detected linear and circular polarisation signals (Hezareh et al., 2013).

Both of these issues will require the partnering of astronomers with experts from the chemical physics community (both at the theoretical and laboratory levels) to be effectively addressed (see for example the case of methanol in Lankhaar et al. 2016).

2.3 Astrochemistry in protoplanetary disks

Protoplanetary disks are test beds for much of our understanding in astrochemistry, and for organic chemistry in particular. Indeed, ALMA routinely detects a plethora of organic species (and unidentified lines) in such environments. These cold astrophysical environments are typically studied by using deuterated molecules that can be used to infer the temperature, density, chemistry, abundances, ionization level, evolutionary stage and thermal history of the disk (Ceccarelli et al., 2014; Millar, 2015). We refer here to W005: Signposts of planet formation in protoplanetary disks, van der Marel et al.

2.4 Exoplanet Atmospheres

Canada is a leader in exoplanet studies, and there is much interest in studying especially exoplanet atmospheres, for instance as a means to find clues about the habitability of the exoplanets (Seager & Deming, 2010; Wakeford et al., 2018). The launch of JWST will open up the window to study these atmospheres in the mid-IR. A big issue here is that our ability to interpret the observations will be limited because we do not currently have a good understanding of the underlying molecular physics (Fortney et al., 2016). Indeed, the spectra of many molecules are incomplete, incorrect or completely unknown, and much theoretical and experimental work will be needed to ready the community for the JWST observations (and for its possible successor, the mid- to far-infrared Origins Space Telescope).

2.5 Identification and modeling of molecular spectral features

Identifying molecules in astronomical observations is another challenge, and the literature is rife with claims about detections, only to be refuted shortly thereafter. Depending on their nature, molecular spectral features appear in different parts of the EM spectrum, and each of them has their own challenges. In the UV and optical, molecules exhibit electronic transitions, and these can be quite complex. Laboratory spectra will produce at least several, but often tens of transitions in a single experiment, and depending on the conditions, they may not all originate from the electronic ground state, and there may be contaminants in the spectrum as well. A critical evaluation of the spectrum typically involves a detailed comparison to computationally obtained electronic energy level structures.

While such computations are not accurate enough to predict frequencies of transitions within a reasonable accuracy, they allow to make the correct assignments for each of the transitions, which in turn can be important to assess coupling with other states (including vibrational and rotational states). The importance of this step became clear recently in the debate about the identification of the C_{60}^+ DIBs. As it turns out, we do not fully understand the complicated coupling between different levels, and this has an effect on the band shapes and on the relative strengths of the bands – key factors that have been traditionally used as criterion to establish an identification as true. There are more reasons why a side by side comparison of astronomical observations and laboratory spectra may not be appropriate. Different laboratory techniques have their own strengths and weaknesses. For instance, Matrix Isolation Spectroscopy offers a quick and cheap way to get an electronic spectrum over a fairly large wavelength range, but it introduces unpredictable shifts and broadening in the resulting spectral lines. A better technique is Cavity Ring-Down Spectroscopy, but this is an expensive and slow technique that can only scan fairly small wavelength ranges at a time, and typically only for fairly small molecules. For large ions, recent techniques have resulted in a breakthrough in the DIB fields, but even there the techniques introduce effects on the details of the spectra that turn out to be important. Given that our astronomical observations typically have a much better resolution and precision than many laboratory measurements, it is important that astronomers educate themselves on the limitations and uncertainties of each technique before comparing to observations.

In the IR, we are primarily looking at vibrational transitions. Laboratory techniques can suffer from similar issues as in the UV/optical, but typically shifts are less pronounced in this range. Here, other issues surface. Even small molecules can have very rich vibrational spectra, and each vibrational transition couples with rotational transitions. Temperatures encountered in outflows of evolved stars or in exoplanet atmospheres are high enough to result in a significant population in myriads of excited states that include overtones and combination bands, and each of these vibrational bands includes a rotational ladder as well. As a consequence, astrophysically relevant line lists often need to include billions of lines (see e.g. Polyansky et al., 2018, for water), and thus detailed line lists developed for the Earth's atmosphere (such as the HITRAN database, Gordon et al., 2017) are not good enough to reproduce the astronomical spectra for higher temperatures or large column densities (as an example for species like C_2H_2 and HCN, see Speck et al., 2006) and consequently we cannot determine good physical parameters from these observations either. The development of these line lists typically involves the analysis of a set of high-resolution laboratory spectra in the gas-phase, to then determine the molecular constants, and accurate energies for the vibrational energy levels and transitions. When this is done carefully and starting from the proper laboratory spectra, it is generally possible to develop a very comprehensive description of all energy levels and descriptions using computational methods. Creating such a line list for a single species is a daunting task, and it takes a good chemistry graduate student in a well-equipped lab often an entire PhD to complete this. For larger molecules, laboratory measurements are often not available, and then astronomers often turn to the output of quantum chemistry computations, and more specifically, to the output of Density Functional Theory (DFT) to predict the wavelengths of the so-called normal vibrational modes. How well this works depends a lot on the molecule that is being studied. In any event, the predicted frequencies need at least to be scaled to match available experimental values, and the infrared intensities are expressed in the somewhat obscure unit of $[km\ mol^{-1}]$. One cannot generally directly compare the output of DFT calculations to astronomical observations, yet that is what happens far too frequently. For large molecules with many vibrational modes, anharmonicities need to be taken into account explicitly as well, since the appearance of overtones and combination bands in the spectra is very clear, and moreover this can result in a re-distribution of the intensities over different modes, thus greatly changing the spectrum. In the far-IR, we would expect to see skeleton modes of large molecules, but no such bands have been detected to date.

In the submm and radio regime, we can probe the pure rotational transitions of molecules. For well-known and abundant species like CO, the frequencies are straightforward to calculate and entire rotational ladders can be observed. However, ALMA observations of protoplanetary disks or evolved stars invariably show a wealth of unidentified features. The challenges in this regime are of a different nature: for a given molecule, we can calculate the frequencies for rotational transitions with some uncertainty, but within that range allowed by the uncertainty, there are often a large number of unidentified lines. Thus, identifying a species based on the pure rotational lines requires a match with a large number of lines. The only way to improve this situation is once more to obtain

state-of-the-art laboratory spectra.

2.6 Details of the molecular physics

A challenge of a very different nature has to do with a good, detailed understanding of the physical processes at the molecular level. Such understanding is necessary to turn molecular features into diagnostic. As a modern example, consider the 2 strongest DIBs due to C_{60}^+ . Observational reports suggest that the ratio of the equivalent widths of these two bands is variable from one sightline to another (Galazutdinov et al., 2017), an effect that was perhaps not expected by most astronomers since both DIBs originate from the electronic ground state. State-of-the-art electronic structure calculations (Lykhin et al., 2019) have offered a possible explanation; if true, the effect is the consequence of different temperatures. Consequently, if this can be confirmed, we can turn measurements of these DIBs into a probe for the local temperature.

The need for a good understanding of molecular astrophysics also surfaces when trying to identify other phenomena, such as the so-called Extended Red Emission (ERE). The ERE represents very efficient photoluminescence by as yet unidentified carbonaceous nanoparticles. The most likely mechanism that can cause the ERE is recurrent fluorescence, also called Poincaré fluorescence (Leger et al., 1988). Recurrent fluorescence can only occur in highly isolated molecules such as is the case for molecules in the ISM where collision timescales are much longer than the timescales for internal molecular processes. Such processes cannot be completely simulated in laboratories, but the viability of the process was demonstrated in the lab nonetheless (Ebara et al., 2016). Understanding such details is also important when considering the limits of laboratory experiments.

3 Recommendations

Molecular Astrophysics and Astrochemistry carry out the essential “under the hood” work that leads to the tools that the greater astronomical community needs to study the Universe. These are interdisciplinary fields and that comes with challenges and opportunities. Within that context, we have the following recommendations:

1. We recommend recognition from the astronomical community for the importance of fundamental work in molecular astrophysics and astrochemistry for a wide range of astrophysics research avenues. This recognition can influence funding decisions, and perhaps funding for facilities could explicitly include a fraction of the funding dedicated to support such research. This is particularly important because the interdisciplinary nature of molecular astrophysics and astrochemistry puts researchers at risk of finding their work not belonging in any of the communities they serve.
2. Building molecular tools requires access to observations at high spectral resolution that cover the electronic, vibrational and rotational transitions of these molecules. We thus recommend that Canada remains strongly involved and invested in state-of-the-art facilities from the near-UV to sub-mm wavelengths.
3. There is currently no easy way to find other researchers interested in molecular astrophysics and astrochemistry in Canada and connect with them. This is most likely the case for other fields as well. It may be useful to organize the various research communities under CASCA’s umbrella somewhat, along the lines of e.g. different AAS Divisions, and have this information be publicly available. This would greatly help researchers (internal and external to CASCA, as could be expected for a highly interdisciplinary field) find their community members across the country, and would allow to direct students who are interested in this field to the right person. Once a community is established, it is also easier to advocate for common causes. We would be happy to organize the molecular astrophysics & astrochemistry community as a first case.
4. We recommend that astronomers actively and explicitly reach out to chemists, molecular physicists, and researchers in other disciplines and engage them for astrophysics research. Such collaborations have proven

very successful elsewhere (e.g. the Dutch Astrochemistry Network, DAN), and allow some molecular astrophysicists to tap into funding streams that would otherwise not be available. A higher visibility for interdisciplinary research may also prove attractive for students from non-astrophysics streams, as has been the case in other countries. One possible roadblock that should be addressed is that entrance requirements (and graduate course requirements) in an astrophysics graduate program may exclude even the best chemistry graduates from molecular astrophysics research.

5. We recommend the creation and distribution to the astronomical community of a set of tutorial-style guidelines and caveats to facilitate a good and reliable comparison between astronomical observations and laboratory experiments or computational spectra.

1: How does the proposed initiative result in fundamental or transformational advances in our understanding of the Universe?

Molecular astrophysics and astrochemistry carry out the work that leads to powerful diagnostic tools that the entire astronomical community uses to study objects and processes in the Universe. The more we understand about the fundamental molecular physics and chemistry, the more powerful these tools will be, and the more complete our understanding of the Universe.

2: What are the main scientific risks and how will they be mitigated?

Development of the tools requires access to good facilities that allow sensitive observations at high spectral resolution from the near-UV to sub-mm wavelengths. A clear risk would be losing access to such facilities.

3: Is there the expectation of and capacity for Canadian scientific, technical or strategic leadership?

Canada has a heritage in molecular spectroscopy, has the observational capacity and some of the world's experts in their ranks that have delivered major contributions to the field. If Canadian astrophysicists can engage researchers from other fields (chemistry, computer science, materials science, molecular physics) then there is an excellent opportunity for international leadership through programs with JWST for instance. This would also allow tapping into streams of funding and students that astronomers would otherwise have no access to.

4: Is there support from, involvement from, and coordination within the relevant Canadian community and more broadly?

The Molecular Astrophysics and Astrochemistry community is spread out across different astronomical fields and across the country, and is not structurally organized. Better coordination is desirable.

5: Will this program position Canadian astronomy for future opportunities and returns in 2020-2030 or beyond 2030?

It will do both.

6: In what ways is the cost-benefit ratio, including existing investments and future operating costs, favourable?

Some funding should be sought to promote this interdisciplinary field, including identifying how best to tap into new funding opportunities. For astronomy, the cost-benefit ratio could well be favourable, since there is the potential to use funding from chemistry, physics and materials science for fundamental and applied astrophysics research.

7: What are the main programmatic risks and how will they be mitigated?

None identified.

8: Does the proposed initiative offer specific tangible benefits to Canadians, including but not limited to interdisciplinary research, industry opportunities, HQP training, EDI, outreach or education?

It is a highly interdisciplinary field, that offers HQP more ways out than staying in astronomy academia, and often a more direct connection to the industry. Experience in other countries has shown that this attracts driven students from a variety of disciplines into astrophysics.

References

- Berné, O., & Tielens, A. G. G. M. 2012, *Proceedings of the National Academy of Science*, 109, 401
- Boogert, A. C. A., Gerakines, P. A., & Whittet, D. C. B. 2015, *ARA&A*, 53, 541
- Cami, J. 2015, *Highlights of Astronomy*, 16, 705
- Cami, J., Bernard-Salas, J., Peeters, E., & Malek, S. E. 2010, *Science*, 329, 1180
- Cami, J., & Cox, N. L. J., eds. 2014, *IAU Symposium*, Vol. 297, *The Diffuse Interstellar Bands*
- Cami, J., Peeters, E., Bernard-Salas, J., Doppmann, G., & De Buizer, J. 2018, *Galaxies*, 6, 101
- Campbell, E. K., Holz, M., Gerlich, D., & Maier, J. P. 2015, *Nature*, 523, 322
- Ceccarelli, C., Caselli, P., Bockelée-Morvan, D., et al. 2014, in *Protostars and Planets VI*, ed. H. Beuther, R. S. Klessen, C. P. Dullemond, & T. Henning, 859
- Cordiner, M. A., Linnartz, H., Cox, N. L. J., et al. 2019, *ApJ*, 875, L28
- Cortes, P. C., Crutcher, R. M., & Watson, W. D. 2005, *ApJ*, 628, 780
- Cox, N. L. J., Cami, J., Farhang, A., et al. 2017, *A&A*, 606, A76
- Ebara, Y., Furukawa, T., Matsumoto, J., et al. 2016, *Phys. Rev. Lett.*, 117, 133004
- Ehrenfreund, P., & Charnley, S. B. 2000, *ARA&A*, 38, 427
- Fan, H., Hobbs, L. M., Dahlstrom, J. A., et al. 2019, *ApJ*, 878, 151
- Fortney, J. J., Robinson, T. D., Domagal-Goldman, S., et al. 2016, *arXiv e-prints*, arXiv:1602.06305
- Fulvio, D., Góbi, S., Jäger, C., Kereszturi, Á., & Henning, T. 2017, *ApJS*, 233, 14
- Galazutdinov, G. A., Shimansky, V. V., Bondar, A., Valyavin, G., & Krelowski, J. 2017, *MNRAS*, 465, 3956
- Goldreich, P., & Kylafis, N. D. 1981, *ApJ*, 243, L75
- Gordon, I., Rothman, L., Hill, C., et al. 2017, *Journal of Quantitative Spectroscopy and Radiative Transfer*, 203, 3, hITRAN2016 Special Issue
- Heger, M. L. 1922, *Lick Observatory Bulletin*, 10, 146
- Hezareh, T., Wiesemeyer, H., Houde, M., Gusdorf, A., & Siringo, G. 2013, *A&A*, 558, A45
- Houde, M., Hezareh, T., Jones, S., & Rajabi, F. 2013, *ApJ*, 764, 24
- Kataoka, A., Muto, T., Momose, M., Tsukagoshi, T., & Dullemond, C. P. 2016, *ApJ*, 820, 54
- Krasnokutski, S. A., Goulart, M., Gordon, E. B., et al. 2017, *ApJ*, 847, 89
- Kroto, H. W., Heath, J. R., O'Brien, S. C., Curl, R. F., & Smalley, R. E. 1985, *Nature*, 318, 162
- Lankhaar, B., Groenenboom, G. C., & van der Avoird, A. 2016, *J. Chem. Phys.*, 145, 244301
- Leger, A., D'Hendecourt, L., & Boissel, P. 1988, *Phys. Rev. Lett.*, 60, 921
- Lykhin, A., Ahmadvand, S., & Varganov, S. 2019, *J. Phys. Chem. Lett.*, 10, 115
- Maragkoudakis, A., Ivkovich, N., Peeters, E., et al. 2018, *MNRAS*, 481, 5370
- Maury, A. J., Girart, J. M., Zhang, Q., et al. 2018, *MNRAS*, 477, 2760
- Millar, T. J. 2015, *Plasma Sources Science Technology*, 24, 043001
- Peeters, E. 2014, in *IAU Symposium*, Vol. 297, *The Diffuse Interstellar Bands*, ed. J. Cami & N. L. J. Cox, 187–196
- Polyansky, O. L., Kyuberis, A. A., Zobov, N. F., et al. 2018, *MNRAS*, 480, 2597
- Riechers, D. A., Pope, A., Daddi, E., et al. 2014, *ApJ*, 786, 31
- Seager, S., & Deming, D. 2010, *ARA&A*, 48, 631
- Speck, A. K., Cami, J., Markwick-Kemper, C., et al. 2006, *ApJ*, 650, 892
- Tielens, A. G. G. M. 2005, *The Physics and Chemistry of the Interstellar Medium* (Cambridge University Press)
- . 2008, *ARA&A*, 46, 289

—. 2013, *Reviews of Modern Physics*, 85, 1021

Wakeford, H. R., Sing, D. K., Deming, D., et al. 2018, *AJ*, 155, 29

Walker, G. A. H., Campbell, E. K., Maier, J. P., & Bohlender, D. 2017, *ApJ*, 843, 56

Zhen, J., Castellanos, P., Paardekooper, D. M., Linnartz, H., & Tielens, A. G. G. M. 2014, *ApJ*, 797, L30