Astronomy in Focus, Volume 1, Focus Meeting 12
XXIXth IAU General Assembly, August 2015
Piero Benvenuti, ed.

doi:10.1017/S174392131600315X

Telescope Observations of Interstellar and Circumstellar Ices: Successes of and Need for Laboratory Simulations

A. C. A. Boogert

Universities Space Research Association, Stratospheric Observatory for Infrared Astronomy,
NASA Ames Research Center, MS 232-11, Moffett Field, CA 94035, USA
email: `acaboogert@alumni.caltech.edu`

Abstract. Ices play a key role in the formation of simple and complex molecules in dense molecular clouds and in the envelopes and protoplanetary disks surrounding young stars. Some fraction of the interstellar ices may become building blocks of comets, and thus be delivered to the early Earth. Laboratory simulations have proven to be crucial in the derivation of ice abundances, in quantifying reaction rates on cold grain surfaces, in determining the thermal and energetic processing history of the ices, and in understanding the interaction between the ices and the underlying refractory grain surfaces. In this invited topical paper I will review possible ways forward in improving our knowledge of the composition of the ices, as many signatures in the interstellar spectra are still poorly identified. I will also emphasize the observed importance of thermal processing of the ices (crystallization, segregation), which likely affects the chemistry after the initial dominance of grain surface reactions. Continued laboratory work is warranted in view of the upcoming observational data from, for example, the *James Webb Space Telescope* (JWST), which is ideally suited for ices studies. For an exhaustive review on this topic I refer to Boogert, Gerakines & Whittet (2015).

Keywords. astrochemistry, stars: formation, ISM: clouds, (ISM:) dust, extinction, ISM: abundances, ISM: molecules, molecular processes, methods: laboratory, infrared: ISM, telescopes

1. Introduction: Ice Formation

Observations of background stars have shown that H_2O and CO_2 ices form at visual extinctions A_V ~1.5 magnitude into dense clouds and cores, where they are shielded from the effects of photodesorption by the interstellar radiation field. Cold grain surface chemistry of O, H, and CO accreted from the gas is the dominant formation process. The intermediate product OH in H_2O formation also reacts with CO to form CO_2, resulting in an intimate mixture of CO_2 and H_2O ices. Deeper into the cloud (A_V ~3 magnitude), the gas becomes molecular (H_2/H increases) and a more volatile (T <10 K) pure CO ice layer is formed. Observations have shown that at even greater depths (A_V ~9 magnitude), at high densities (10^5 cm^{-3}), CO ice hydrogenation leads to CH_3OH. The resulting mixture of CH_3OH with CO can be spectroscopically traced by a long wavelength wing of the 4.67 μm CO ice band. Penteado *et al.* (2015), expanding on work by Cuppen *et al.*(2011), show that the strength and shape of this wing agree with the strength and shape of the 3.53 and 9.7 μm bands of CH_3OH, as well as the ^{13}CO ice band toward the massive YSO AFGL 7009S. A gradient in mixing ratios of CO:CH_3OH=1:1-1:9 is possible, reflecting varying CH_3OH formation efficiencies over time.

2. Further Constraints on the Composition of Interstellar and Circumstellar Ices

The easily identifiable, strong modes of several simple ice species (CO, H_2O, CO_2, CH_3OH) are well studied. Absorption profile variations in samples of background stars and Young Stellar Objects (YSOs) are related to variations of the composition and the thermal history of the ices. These ice bands indeed have diagnostic value as to the nature and physical history of the line of sight observed. A number of absorption features are still not reliably identified, however. This is primarily because the infrared wavelength range traces vibrational modes of functional groups, e.g., the C-O stretch and N-H bending modes, which occur at similar wavelengths for different molecular species. Further observational constraints are possible, however, as the spectral resolving power of *Spitzer Space Telescope* observations in the 5-8 μm wavelength range is very low ($R = \lambda/\Delta\lambda \sim 60-100$). In particular for the distinct 7.25 and 7.41 μm ice features, the much improved spectral resolution of JWST ($R \sim 3000$) at two orders of magnitude better sensitivity will allow much more accurate measurements of the absorption profiles for much larger samples of sightlines (these features were so far reported in just a handful of sightlines). For the same reasons, further observational constraints can be expected for the elusive 6.85 μm ice band, the 7.58 μm "SO_2" band, and signatures of PAH species embedded in the ices.

A different approach to further constrain the composition of the ices is by measuring the ice lattice and torsional modes. These are more unique identifiers of specific molecules than the mid-infrared vibrational modes, as laboratory experiments have shown (e.g., Ioppolo *et al.* (2014)). The required telescope instrumentation, low-resolution spectrometers with wide instantaneous band-width and accurate broad-band spectral response calibration, are not available, however. This is a niche for future instruments on the *Stratospheric Observatory for Infrared Astronomy* (SOFIA).

3. Processing of Interstellar and Circumstellar Ices

In dense clouds and circumstellar environments, grain surface chemistry sets the bulk ice composition. Subsequently, thermal and energetic processing are expected to modify the ices. In particular, laboratory simulations have shown that energetic radiation (ultraviolet photons) and particles (cosmic rays) break molecular bonds and the radicals form more complex species. This has been hard to prove observationally however. Thermal processing on the other hand, is easily observed by the spectroscopic effects of crystallization, segregation, and sublimation. Considering the prominence of such heated ices in the envelopes and disks of YSOs, one must consider the efficiency of purely thermal reactions. For example, laboratory mixtures of H_2CO with NH_3 show an efficient formation of polyoxymethylene (POM), a polymer of the CH_2O group (Schutte *et al.* (1993)). The same mixture yields aminomethanol (NH_2CH_2OH), and the energy barriers and rates of this and other purely thermal reactions were measured by Theulé *et al.* (2013).

References

Boogert, A. C. A., Gerakines, P. A., & Whittet, D. C. B. 2015, *ARAA*, 53, 541

Cuppen, H. M., Penteado, E. M., Isokoski, K., van der Marel, N., & Linnartz, H. 2011, *MNRAS*, 417, 2809

Ioppolo, S., McGuire, B. A., Allodi, M. A., & Blake, G. A. 2014, *Faraday Discuss.*, 168, 461

Penteado, E. M., Boogert, A. C. A., Pontoppidan, K. M., *et al.* 2015, *MNRAS*, 454, 531

Schutte, W. A., Allamandola, L. J., & Sandford, S. A. 1993, *Icarus*, 104, 118

Theulé, P., Duvernay, F., Danger, G., *et al.* 2013, *Adv. Sp. Res.*, 52, 1567