

INVITED TALK

NASA LAW, February 14-16, 2006, UNLV, Las Vegas

## A brief summary of some of the laboratory astrophysics workshop

William Klemperer

*Department of Chemistry, Harvard University, Cambridge, MA 2138*

klemperer@chemistry.harvard.edu

Our present knowledge of the molecular universe has come primarily from radio observations [ I include here millimeter and submillimeter in this rubric]. There are a number of reasons for this but the primary one is the extremely high spectral resolution. The ease of observing emission from the volume of dense molecular clouds without significant attenuation by scattering from dust has shown this to be the powerful observational tool for molecular astronomy. Finally the relative simplicity of rotational compared to vibrational or electronic spectroscopy allows carrier identification as well as facile evaluation of cloud conditions such as density and temperature.

These virtues become tenuous as the astronomical observations are pushed to higher frequencies for enhanced observational sensitivity. Thus precision rest frequencies are mandatory for the search for new species. We may inquire about which new species require particular attention, and which species may be relatively safely predicted on the basis of lower frequency laboratory measurements. For a **rigid** rotor the three rotational constants are sufficient to completely specify the transition frequencies. The intensities require the three components of the electric dipole moment. For semirigid species, where the centrifugal distortion, may be treated at the quartic level of angular momentum (Bunker et al. 1998), up to five additional constants are required (Watson 1967). There are a number of such species of considerable interest, where laboratory measurements are adequate for astronomical searches. A most interesting species in this class is corannulene (Lovas et al. 2005),  $C_{20}H_{10}$ , an extremely rigid polar polyaromatic hydrocarbon, with oblate symmetric rotor structure. The important centrifugal distortion constant  $D_{JK}$  is vanishingly small, thus the spectrum is essentially that of a linear molecule. The present limits on its abundance may be set as less than . Further the semi-rigid polar heterocyclic aromatic species furan, pyrrole, and pyridine have been well studied (Townes & Schawlow 1975). Thus far they have not been observed in the interstellar medium.

The third type of species are those with large amplitude internal motions. These are both interesting since they include molecules that are frequently regarded biologically relevant. Of these glycine is an model example. The adequacy of the semi-rigid rotor discussed above is highly doubtful. Thus low frequency measurements (Kuan et al. 2003) do not allow reliable prediction of higher frequency transitions (Snyder et al. 2005) when the crowded nature of the millimeter spectrum of rich regions such as Sag B2 and OMC1 is considered. While it

is transparently obvious that precision laboratory frequency measurements for each spectral region to be studied will reduce ambiguity in this problem, it is highly desirable to develop accurate higher order theory for species with large amplitude internal motions. This will be interesting in its own right but may provide more reliable methods of extrapolation to higher frequencies. There has been a considerable progress in treating large amplitude motions of weakly bound species (Bunker et al. 1998; Kozin et al. 2004). The ability to execute large numerical calculations in terms of the molecular potential provides a new means to estimate higher energy levels and transitions from fitting of lower ones. The question of how well one can theoretically extrapolate low frequency transitions of non-rigid to the relevant high frequency regions is both interesting and of broad interest.

A second area in which a considerable progress could be achieved is that of plasmas. There is a huge effort, primarily by the Department of Energy in fusion plasmas. This effort is generally a heavily directed large scale engineering one. The scientific content remains low. On the other hand the plasmas play an extremely important role astrophysically. The subject is extremely rich intellectually. There appears to be a wall between these efforts. In this writers opinion the Department of Energy would be wise in investing in basic research of astronomical plasmas.

The power of chemical models for interstellar and circumstellar regions has been well documented. In pushing forward there are many questions in which laboratory astrophysics will be extremely valuable if not essential. First are the rates of ion molecule processes at typical dark cloud temperatures, 10 K. Of primary concern is the direct measurement of radiative association rates well illustrated by the important reaction  $\text{CH}_3^+ + \text{H}_2 \rightarrow \text{CH}_5^+ + \text{photon}$  (Barlow, Dunn, & Schauer 1984). Since for gas phase reactions determination of reaction cross section allows facile application to interstellar modeling this area is one of high payoff. A further question along these lines is whether there are quantum state selectivity in hydride reactivity. The ubiquitous  $\text{CH}^+$  remains of considerable interest especially in translucent clouds, where it is observed in the  $J = 0$  level. Can its reactivity in this level be different than in higher rotational levels?

The importance of surface reactions is clear with the recombination of atomic hydrogen occurring on grains. The treatment of this process is important, and apparently not a simple rate equation. The abundance of atomic hydrogen in dark molecular clouds is likely important for a number of reactions. The treatment of the hydrogen recombination avoids the many questions of surface chemistries at 10K such as will reaction products desorb from the cold surface.

## REFERENCES

- Bunker, P. R., & Jensen, P. 1998, Chap. 13, Molecular Symmetry and Spectroscopy, 2nd Edition, National Research Council Canada

- Watson, J. K. G. 1967, *J. Chem. Phys.*, 46, 1935
- Lovas, F. J., McMahon, R. J., Grabow, J.-U., Schnell, M., Mack, J., Scott, L. T., & Kuczkowski, R. L. 2005, *J. Am. Chem. Soc.*, 127, 4345
- Townes, C. H., & Schawlow, A. L. 1975, *Microwave Spectroscopy* (Dover)
- Kuan, Y.-J., Charnley, S. B., Huang, H.-C., Tseng, W.-L., & Kisiel, Z. 2003, *ApJ*, 593, 848
- Snyder, L. E., Lovas, F. J., Hollis, J. M., Friedel, D. N., Jewell, P. R., Remijan, A., Ilyushin, V. V., Alekseev, E. A., & Dyubko, S. F. 2005, *ApJ*, 619, 914
- Bunker, P. R., & Jensen, P. 1998, Chap. 16, *Molecular Symmetry and Spectroscopy*, 2nd Edition, National Research Council Canada
- Kozin, I. N., Law, M. M., Tennyson, J., & Hutson, J. M. 2004, *Computer Physics Communications*, 163, 117
- Barlow, S. E., Dunn, G. H., & Schauer, M. 1984, *Phys. Rev. Lett.*, 52, 902