EXOMOL: MOLECULAR LINE LISTS FOR EXOPLANET AND OTHER ATMOSPHERES

J. TENNYSON, R. J. BARBER, A. AZZAM, M. DOWN, and C. HILL, *Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK*; S. N. YURCHENKO, *Technische Universität Dresden, Physikalische Chemie, D–01062 Dresden, Germany*.

Spectral characterization of astrophysical objects cool enough to form molecules in their atmospheres (cool stars, extrosolar planets and planetary discs) requires considerable amount of fundamental molecular data. The existing molecular line lists (with some exceptions) are however not sufficiently accurate and complete. We present a new (five years) European Union project ExoMol aimed at bridging this gap: ExoMol will generate comprehensive line lists for *all* molecules likely to be observable in exoplanet atmospheres in the foreseeable future. This is a huge undertaking which will mean providing in excess of 10^{11} spectral lines for a large variety of molecular species.
The physics of molecular absorptions is complex and varies between different classes of absorbers. The project will therefore be divided into following topics (a) diatomic, (b) triatomics, (c) tetratomics, (d) methane and (e) larger molecules. Each of which will require special techniques will be required in each case. The majority of diatomic systems to be tackled are open shell species involving a transition metal atom; the opacity is provided by the transitions between the many low lying electronic states of the system. The calculation of rotation-vibration line lists for closed-shell triatomic systems is now relatively straightforward provided enough care is taken in deriving the potential energy surface. For H_2S calculations are in progress: the unusual properties of the dipole moment will also require careful treatment. Accurate rotation-vibration line lists for hot tetratomic molecules such as ammonia, acetylene, hydrogen peroxide and formaldehyde, are at the very limit of what is computationally possible at present. These will be computed either by direct calculation of the full line list, such as our hot ammonia line list BYTe developed recently [S. N. Yurchenko, R. J. Barber , and J. Tennyson, *Mon. Not. R. Astron. Soc., in press*, (2011)], or by use of high accuracy vibrational calculations onto which the rotational structure will be grafted using ideas developed from the standard perturbation theory approach to molecular spectroscopy. Tests for acetylene suggest that this latter approach, although intrinsically less accurate, is still able to give reliable results [A. Urru, I. N. Kozin, G. Mulas, B. J. Braams, and J. Tennyson, *Mol. Phys.*, **108**, 1973 (2010)]. Data from this project can be accessed at www.exomol.com.