

Infrared relaxation in Hydrogenated Amorphous Carbon Chemical Analogues

G. Molpeceres,¹ B. Maté,¹ J. Ortigoso¹ and H.A Galué²

¹Departamento de Física Molecular, IEM-CSIC., *Spain*

²Department of Physics and Astronomy, Vrije Universiteit, *Netherlands*

For the past 30 years, Polycyclic Aromatic Hydrocarbons (PAHs) have been able to reproduce the Unidentified Infrared Emission (UIE) emission bands, a set of spectroscopic features found between 11.2 and 6.2 μm and at 3.3 μm in the mid IR, corresponding to aromatic C=C stretchings and bendings and C-H bendings, respectively [1,2]. The so-called PAH hypothesis is able to account for the general appearance of the bands explaining them as a combination of PAHs molecules in different oxidation states [1]. One of the main advantages of PAH molecules is that they can undergo transient heating to effective temperatures of 1000K upon absorption of a single UV photon, relaxing afterwards. With the years, refinements of the classical theory have been developed and successfully applied to the fitting of astronomical sources [3,4]. Several criticisms arise from the classical PAH hypothesis, being the most important one that no single PAH molecule has been positively identified in the Interstellar Medium (ISM) [5]. Among the years, several alternatives have been postulated like considering small solid particles as candidates for carriers of such band and assuming that isolated aromatic domains within these particles may suffer transient heating by UV photons [6,7]. The present work is devoted to the simulation of the UV absorption and IR emission spectra of a series of randomly packed hydrogenated amorphous carbon (HAC) chemical analogues [8] using ab initio methods. We have employed CASTEP [9] for the calculation of the vibrational properties and the optical constants in the ultraviolet and visible range. The calculation of the emission curves has been done implementing a canonical photocooldown emission model from the literature [4 and references therein]. We show that the IR photo-cooldown of our randomly packed amorphous analogs is consistent with the spectral characteristics of the interstellar UIE bands, offering a reconciling scenario between the PAH hypothesis and the mixed aliphatic-aromatic amorphous solid interpretations.

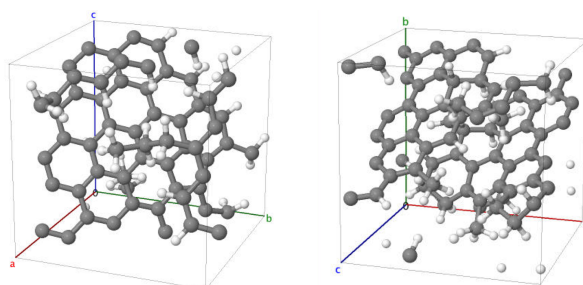


Figure 1: Examples of the packed structures simulated in this work.

References

- [1] Allamandola, L.J, Tielens, A.G.G.M and Barker, J.R 1985 ApJ Letters, 290, p. L25-L28.
- [2] Tielens, A. G. G. M. 2008. Annual Review of Astronomy and Astrophysics, 46(1).
- [3] Rosenberg, M.J.F, Berné, O. and Boersma, C. 2014 A&A 566, L4.
- [4] Galué, H.A., Díaz Leines, G. 2017 PRL 119, 171102.
- [5] Kwok, S. and Zhang, Y. 2013 ApJ, 771, 5.
- [6] Scott, A., Duley, W. and Jahani.H 1997 ApJ 2, L175-L177
- [7] Kwok, S. and Zhang, Y. 2011 Nature, 479, 80-83.
- [8] Molpeceres, G., Timón, V, Jiménez-Redondo, M., et al 2017 PCCP, 19, 1352-1360
- [9] Clark, S. J., Segall, M. D., Pickard, C. J., et al. 2005 Z. Kristallogr, 220, 567–570.

