CHARACTERIZATION AND FORMATION PROCESSES OF C_4^-, C_4H and C_4H^-

M.L. SENENT, *Departamento de Astrofísica Molecular e Infrarroja, Instituto de Estructura de la Materia, C.S.I.C., Serrano 121, Madrid 28006, SPAIN*; V. BRITES, M. HOCHLAF , *Universitè Paris-Est, Laboratoire de Modèlisation et Simulation Multi Echèlle, MSME FRE 3160 CNRS, 5 boulevard Descartes, 77454 Marne-la-Vallèe, FRANCE.*

Using state-of-the-art theoretical methods, we investigate the stable isomers of C_4^-, C_4H and C_4H^-. Three of them are relevant for astrophysics and astrochemistry. These computations are performed using interaction configuration ab initio methods and the aug-cc-pVXZ (X=T,Q) basis sets. In addition to the linear isomers, we predict the existence of several cyclic and branched forms for these molecules. For all the molecular species of interest here, sets of spectroscopic parameters are determined with perturbation theory, which compare quite well with experiment. For $l - C_4H^-(X^1\Sigma^+)$, the quartic force field is computed at the coupled cluster level of theory. This force field is derived from full nine-dimensional potential energy surface generated close to the equilibrium geometry of this anion. Finally, we treat the photochemistry processes of the hydrogen attachment and the electron attachment reactions that may lead to the formation of the C_4H^- from either C_4^- or C_4H.