

MRCI/CASSCF study of the structures and spectroscopic properties of C_3 , C_3H^+ and C_3H

M.L.Senent and Y.G.Smeyers, I.E. de la Materia, C.S.I.C., Serrano 113b, Madrid 28006, SPAIN
Imtls2c@pinar2.csic.es

A.Pérez-Ortega, Facultad de Químicas, UBU, Burgos 09001, SPAIN

R.Domínguez-Gómez, Departamento de Ingeniería Civil, E.U.I.T.O.P., Universidad Politécnica de Madrid, Alfonso XIII, 3-5, Madrid 28014, SPAIN

In this paper, we study the molecular stable geometries and some spectroscopic properties of C_3 , C_3H^+ and C_3H with ab initio calculations at the MPX (X= 2, 3, 4), CASSCF and MRCI levels using extended basis set. The main purpose of the work is the determination of the vibrational levels corresponding to the large amplitude motions. The potential energy surfaces for the lowest electronic states are calculated close to the equilibrium structures. C_3 and C_3H^+ ground electronic state are singlet states preserved during the protonation process. The ground electronic state of C_3H is a $^2\pi$ doubly degenerate. This radical present strong Renner-Teller vibronic effect that requires non-conventional Hamiltonians for the determination of the spectral lines.