MILLIMETER WAVE, INFRARED AND AB INITIO STUDY OF FPS

HELMUT BECKERS, HANS BÜRGER, PETER PAPLEWSKI, *Anorganische Chemie, FB 9, Universität-GH, D-42097, Wuppertal, Germany*; JÜRGEN BREIDUNG, WALTER THIEL, *Max-Planck-Institut für Kohlenforschung, D-45470 Mülheim an der Ruhr, Germany*; MARCEL BOGEY, PASCAL DREAN and ADAM D. WALTERS, *Physique des Lasers, Atomes et Molécules, Centre d'Etudes et de Recherches Lasers et Applications, Université des Sciences et Technologies de Lille, F-59655 Villeneuve d'Ascq, France*.

We show how a collaborative study involving ab initio calculations, chemistry, rovibrational spectroscopy and pure rotational spectroscopy can successfully be used to predict, produce, identify and characterize new short-lived molecular species. Ab-initio calculations at the MP2 and CCSD(T) level with VQZ1+ basis set were carried out using GAUSSIAN98 and MOLPRO98 programs in Mühlheim. FPS was produced by pyrolysis of F_2PSPF_2 synthesized at Wuppertal and the rotationally resolved ν_1 band then identfied by FTIR spectroscopy. Accurate rotational and centrifugal distortion constants in the ground state were determined using millimeter wave spectroscopy in Lille. Measurements of the ^{34}S isotopomer and ν_3 vibrationally excited state will allow an experimental approximation to the equilibrium structure.