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MSI2H2+ STRUCTURE (M: CR, MN AND W) THEORETICAL AND FT-IRC MASS SPECTROMETRY STUDY

A Ferhati

LCCE-Université de Batna, Algérie

Progress has been made in the knowledge of the nature of the M-X bonding (M=Cr, Mn and W; X=C, Si...) both experimentally and theoretically. A Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) study of the gas phase reaction I of M+ with SiH4 is reported here in order to give more insight on the structure of the MSi2H2+ ion

M++ 2SiH₄->MSi₂H₂*+₂H₂ (I)

The structure of the MSi2H2+ ions are discussed in terms of CID result confronted to the theoretical calculation at the DFT level on the different structural geometries.

ferhati_azedine@hotmail.com azeddine.ferhati@univ-batna.dz



Figure 1: WSi2H2+ CID spectra obtained with 17 eV collision energy