Conformational stabilities of CH2=CHSi(CH3)(n)X3-n (X = F and Cl) from variable temperature FT-IR spectra of rare gas solutions

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Abstract: Variable temperature (-105 to - 150 degreesC) studies of the infrared spectra (3500-400 cm(-1)) of methylvinyldifluorosilane, CH2CHSiF2CH3, dimethvlvinylfluorosilane CH2CHSiF(CH)(2) and methylvinyldichlorosilane, CH2CHSiCl2CH3, dissolved in liquid krypton have been recorded. The enthalpy difference of methylvinyldifluorosilane has been determined to be 53 +/- 11 cm(-1) (0.64 +/- 0.13 kJ/mol) with the gauche conformer the more stable form. However in the crystalline solid only the cis conformer is present. For the corresponding dichlorosilane the enthalpy difference has been determined to be 46 +/- 20 cm(-1) (0.55 +/- 0.23 kJ/mol) with the cis conformer more stable. For dimethylvinylfluorosilane the enthalpy difference has been determined to be 32 +/- 7 cm(-1) (0.38 +/- 0.08 kJ/mol) with the gauche conformer the more stable form, Ab initio calculations have been carried out with several different basis sets up to MP2/6-311 + G(2d,2p) with full electron correlation by the perturbation method for all three of the silanes from which the conformational stabilities have been determined.