CONFORMATIONAL STABILITY OF $CH_3CH_2P(Z)F_2$ (Z=O, S) FROM TEMPERATURE DEPENDENT FT-IR SPECTRA OF RARE GAS SOLUTIONS AND r_o STRUCTURAL PARAMETERS

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Variable temperature (-55 to -150°C) studies of the infrared spectra (3500 to 400 cm^{-1}) of ethylphosphonic difluoride, $CH_3CH_2P(O)F_2$ and ethylphosphonothioic difluoride, $CH_3CH_2P(S)F_2$ dissolved in liquid xenon or krypton have been recorded. From these data, the enthalpy differences have been determined to be 76±9 cm^{-1}(0.91±0.11 kJ/mol), for $CH_3CH_2P(O)F_2$ with the trans conformer the more stable rotamer and 53±7 cm^{-1}(0.63±0.08 kJ/mol) for $CH_3CH_2P(S)F_2$ but with the gauche conformer the more stable form. Complete vibrational assignments are presented for both molecules, which are consistent with the predicted frequencies obtained from the ab initio MP2/6-31G(d) calculations. The optimized geometries, conformational stabilities, harmonic force fields, infrared intensities, Raman activities, and depolarization ratios have been obtained from RHF/6-31G(d) and/or MP2/6-31G(d) ab initio calculations. These quantities are compared to the corresponding experimental quantities when appropriate as well as with some corresponding results for some similar molecules. The r_o adjusted structural parameters have been obtained for both molecules from a combination of the microwave rotational constants and ab initio predicted parameters. The corresponding r_o structural parameters have been obtained for some similar molecules for comparison.