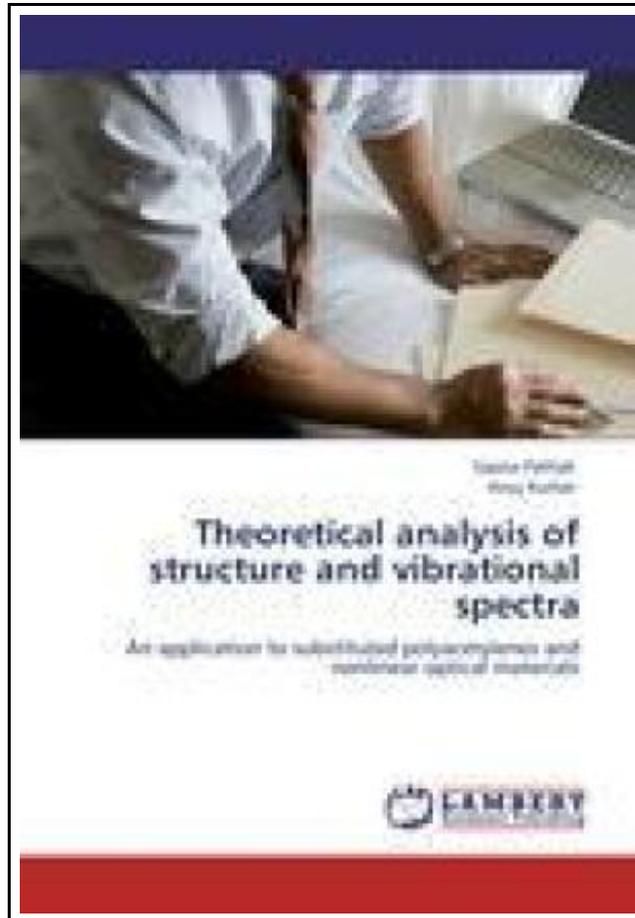# Theoretical analysis of structure and vibrational spectra

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