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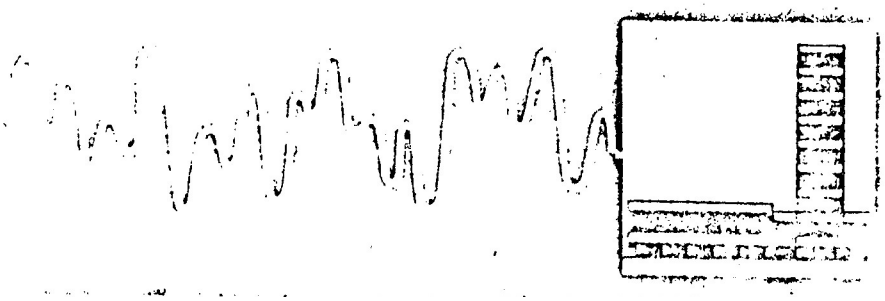
ABSTRACTS



109 INFRARED AND RAMAN SPECTRA AND FREQUENCY CALCULATION OF 2,2'-BIPYRIDYL §

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Single crystals of 2,2'-bipyridyl suitable for infrared and Raman measurements have been grown from the melt. Polarized light Raman spectra have been run gathering the excited light at a 90° configuration and keeping the analyzer in a fixed position in order to get rid of the polarization anomalies of the spectrometer. The crystal structure of 2,2'-bipyridyl is $P2_1/c, (C_{2h}^5)$, so that the tensor elements of the Raman scattering tensor which differ from zero are aa,bb,cc, and ac for totally symmetric A_g modes and ab and bc for b_g modes. All the external lattice modes which are Raman active were identified and assigned to the proper factor group species. Almost all the internal mode splittings have been also identified both in Raman and IR spectra. Different atom-atom potentials of the Buckingham type have been checked for their ability reproducing the crystal structure. All of them brought to minima which only slightly differed from the experimental one. Although very different trial structures have been devised as starting points of the minimization procedure in every cases we had convergence pratically to the same minimum. The lattice modes were calculated using the previous potentials and the experimental crystal coordinates. The agreement with the measured values was fairly good for some modes and poor for others. The calculation was performed in the rigid body approximation so that the discrepancies could originate from the mixing of the internal and external modes which have been ignored in our calculation. Calculation which will take into account the mixing of the modes are in progress as it is the search for a new potential which could better reproduce the experimental structure and frequencies.

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