Inelastic neutron scattering (INS) spectrum of tetracyanoquinodimethane (TCNQ).

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Streszczenie

The vibrational spectra of tetracyanoquinodimethane (TCNQ) in the solid state were studied using the inelastic neutron scattering (INS) technique. The detailed analysis of INS spectra showed advantages of this technique, particularly when analyzing the low frequency (below 1200 cm^{-1}) region. The INS as well as Raman and infra-red (IR) spectra were compared with simulated ones using the Gaussian 98, Gamess and auntieClimax programs. All internal low frequency modes predicted by the calculations were well manifested. One observed an excellent agreement between experimental and calculated INS band intensities. The problem of the frequency scaling factor and an appearance of the summation frequencies was discussed.

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