

OPTICAL VIBRATION SPECTRA OF C_{24}
AND C_{48} CAGE CLUSTERS AND SIMPLE
CUBIC FULLERITE

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S u m m a r y

An analysis of the structure of a new carbon phase, namely, ‘cubic graphite’, has been carried out by optical spectroscopy and computer simulation. Computer simulation results of IR and Raman spectra of carbon cage clusters C_{24} and C_{48} are presented. Calculations have been performed by the spin-restricted Hartree–Fock (RHF) method with the 6-31G(d) basis set. We present the experimental Raman spectra of samples of carbon crystals of the cubic system referred to as cubic graphite in the frequency range 50–3500 cm^{-1} , where the new bands of carbon materials were observed in the frequency range 600–800 cm^{-1} . The analysis of the most intense calculated normal vibrations and the new experimentally detected bands has shown that the location of experimental bands correlates well with that for the theoretically calculated spectrum of cluster C_{24} .