The structure of melanophlogite (46SiO2.6M14.2M12): Simulation of the host framework (M14=M12=0)

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The temperature dependences of the host framework structure of mineral melanophlogite (46SiO2.6M14.2M12) were studied with the aid of the molecular dynamic simulation technique (MDS) at 11 values of temperatures ranging from 50 K to 1200 K. The major results of the present constant temperature and pressure MDS calculations are as follows: (1) The MDS cell edge lengths at 500 K were about 5% shorter than the X-ray value, at 473 K, of Gies (1983), (2) The unit cell was not cubic below about 1000K, (3) The space group symmetry was not Pm-3n, but P-43n at 1200K and (4) Phonon spectra characteristic of quartz also appeared in the power spectral density functions for the present MDS framework structure.