Quantum Monte Carlo determination of the equation of state of cubic boron nitride K.P. ESLER, B. MILITZER, R.E. COHEN, Carnegie Institution of Washington — The pressure inside a diamond anvil cell is usually determined by measuring the pressure-dependent frequency shift of a small ruby sample or by x-ray diffraction on a small chip of a pressure standard. However, there are no primary pressure standards for the megabar range. Recently, cubic boron nitride (cBN) has been suggested as an accurate pressure gauge. Unlike ruby, its structure is highly constrained by symmetry and stable beyond 100 GPa, and it has a well-separated Raman spectrum with sufficient pressure dependence to allow accurate pressure calibration. Its use as a pressure standard requires reliable equation of state (EOS) data. A density functional theory (DFT) calculation of the cBN EOS based on the generalized gradient approximation agrees well with experiment up to 100 GPa, but a calculation that does not depend on an approximate exchange-correlation functional would be desirable. Quantum Monte Carlo (QMC) is a correlated, first-principles simulation method with fewer uncontrolled approximations than DFT methods. We present the results of applying state-of-the-art QMC methods to the bulk cBN solid in order to determine the EOS.