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Ab initio thermodynamics of MgSiO3 protoenstatite at high temperatures conditions

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Protoenstatite (PEn) is one of the high temperature forms of MgSiO3 pyroxenes, having stability range from 1200 to 1600 K at ambient pressure. Its importance has been recognized by many authors, in fact PEn is regarded as a precursor phase of low-clinoenstatite (LP-CEn)/orthoenstatite (OEn) intergrowths in some cometary samples [3] and in calcium-aluminum-rich inclusions (CAIs) from CV3 chondrites [1]. The presence of a high temperature PEn precursor in planetary materials implies that its formation must have occurred close to solar nebula conditions by equilibrium condensation via a reaction between forsterite and gaseous SiO [2] or, alternatively, as a result of reheating process after primary condensation [1]. Despite its role as a precursor mineral phase in the solar system, very little is known about the thermodynamics and phase relations of PEn with other MgSiO3 polymorphs. This is due for the most part to its unquenchable nature, meaning that even if PEn can be synthetized at high temperature conditions, it doesn't preserve as a metastable phase at ambient conditions since it very rapidly reverts either to OEn or LP-CEn [4]. The impossibility to perform measurements on samples of PEn prevents to obtain information on its thermodynamic properties, which are in turn fundamental for the investigation of phase equilibria. In that sense, ab initio calculations based on quantum-mechanical theory are one of the most reliable methods available to obtain information on thermodynamics and phase relations of minerals at planetary conditions. We present a DFT based ab initio B3LYP computational study on MgSiO3 protoenstatite thermodynamics. All the relevant thermophysical and thermodynamic properties of PEn (e.g. heat capacity, vibrational entropy, thermal expansion, EoS) have been calculated in the framework of the quasi-harmonic approximation (QHA) by a full phonon dispersion calculation. This allowed to obtain original insights into protoenstatite thermodynamics and enabled to retrieve a complete set of physically consistent thermodynamic properties, that are in excellent agreement with the very few experimental data currently available.

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