# Equation of state of orthoferrosilite at pressure up to 15 GPa and high temperatures

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Mg- and Fe-pyroxenes are most abundant phases in the Earth's crust and the upper mantle. Therefore, knowledge of their stability and thermodynamic properties is necessary for correct modeling of mantle substance and phase boundaries at the depth at relevant temperatures and pressures. Ferrosilite ($FeSiO_3$) is the ferrous end-member mineral of pyroxene group. There are three $FeSiO_3$-polymorphs observed at ambient *P-T* conditions. Orthoferrosilite (OrthoFs) crystallizes in orthorhombic structure (space group *Pbca*) at ambient pressure and temperature higher 800 K. At ambient temperature and pressure above 4.2 GPa, natural OrthoFs transforms into high-pressure clinoferrosilite (HP-CFs, *C2*/*c*) [1]. The monoclinic phase of low-pressure clinoferrosilite (LP-CFs, $P2_1/c$) forms at standard conditions and upon decompression of HP-CFs phase [2]. Recently, further transition of *C2*/*c* structure to high-pressure $P2_1/c$-phase was detected at pressure range of 30–36 GPa by X-ray diffraction [3]. Thus, a phase diagram topology of the $MgSiO_3$ and $FeSiO_3$ systems is similar, but the phase boundaries of Fe-silicates are shifted to a lower pressure range [4].

We used modified thermodynamic formalism from [5] based on the Helmholtz free energy and constructed the equation of state of $FeSiO_3$-orthoferrosilite. The fitting parameters of equations of state are derived by least squares method in Microsoft Excel by analogy with our study [6]. The features of equation of state of $FeSiO_3$ is magnetic contribution to the Helmholtz free energy. This term is allowed to describe a magnetic transition in the structure of mineral. The obtained parameters of equation of state of orthoferrosilite are as follows: $U_0$ = –1233.81 kJmol$^{-1}$, $V_0$ = 32.95 cm$^3$mol$^{-1}$, $K_0$ = 101.7 GPa, $K'$ = 6.86, $\Theta_{o1}$ = 949.6 K, $m_{1=2}$ = 7.5, $\Theta_{o2}$ = 262.3 K, $\gamma_0$ = 0.952, $\beta$ = 0.587, $a_0$ = 56.26*10$^{-6}$ K$^{-1}$, $m$ = 1, $B_0$ = 0.622, $p$ = 0.28. The calculated heat capacity of OrthoFs is shown on Fig.1.

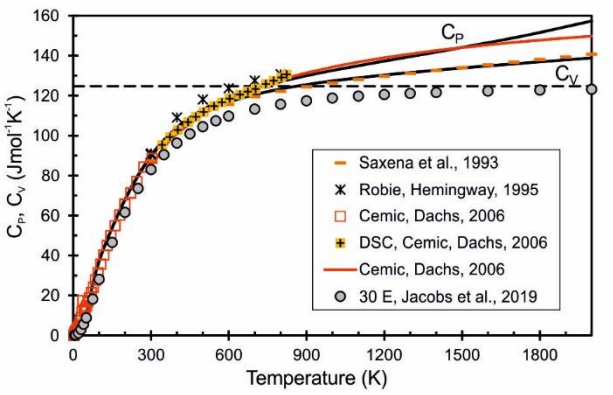


*Figure 1*. Calculated heat capacity of orthoferrosilite in comparison with experimental data and other calculations

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