A new composition-dependent equation of state for clinopyroxene

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Thermodynamic modelling has become a widely employed tool in petrology, geochemistry and geodynamics. Such modelling requires realistic composition-dependent equations of state (*x*-eos) for minerals of petrological interest. Clinopyroxene (cpx) is a common phase in the Earth's mantle and mafic- to intermediate lithologies. There are currently several calibrated *x*-eos for cpx, available for calculations in phase equilibrium software packages such as Perple_X and THERMOCALC. The various *x*-eos are calibrated in different regions of pressure-temperature—composition (P—T—$\mathbf{x}$) space. However, these *x*-eos are not thermodynamically consistent with each other, and therefore cannot be used in the forward modelling of processes that encompass more than one of these regimes.

We are developing a single *x*-eos to represent cpx in common crustal and uppermost-mantle environments, built on the Holland & Powell (2011) dataset [1]. The first step was to amalgamate, as far as possible, the structures and parameterisations of the existing *x*-eos for omphacitic cpx [2], low-pressure, low-Na supra-solidus cpx with significant tetrahedral Al [3] and mantle cpx at < 50 kbar [4]. Next, we must reconcile their inconsistencies by recalibrating against the data originally used in their calibration. Further, we have added high-pressure, low-temperature data (e.g. [5]) to this database that was not used in previous calibrations. The resulting *x*-eos will be suitable for large-scale integrated thermodynamic/geodynamic simulations spanning a wide range of crustal and upper mantle conditions and compositions.

[1] Holland & Powell (2011) *J Metam Geol* **29**, 333-383. [2] Green *et al*. (2007) *Am Min* **92**, 1181-1189. [3] Green *et al*. (2016) *J Metam Geol* **34**, 845-869. [4] Holland *et al*. (2018) *J Petrol* **59**, 881-900. [5] Poli (1993) *Am J Sci* **293,** 1061-1107.