EosFit-Pinc: a GUI program to calculate pressures in host-inclusion systems

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A remnant pressure in an inclusion trapped inside a host mineral is developed because the inclusion and the host have different thermal expansion and compressibilities, and the inclusion does not expand in response to P and T as would a free crystal. Instead it is restricted to expand only as much as the cavity of the host mineral, and this constriction in volume can result in inclusions exhibiting over-pressures when the host is studied at room conditions. The remnant pressure of the inclusion, measured by X-ray diffractometry, birefringence analysis or Raman spectroscopy, can then be used with the equations of state (EoS) of the host and inclusion to constrain the P and T at entrapment. This concept has been known for a long time, but satisfactory quantitative modelling of inclusion-host systems based on non-linear elasticity theory and precise EoS has only recently come available (Angel et al., 2014, 2015), even though calculations still assume isotropic elastic properties.

The elasticity calculations to determine entrapment conditions involving the EoSs for both the host and the inclusion are complex if thermodynamically-realistic EoS are employed. We have therefore developed a simple GUI program, EosFit-Pinc that performs all of the necessary calculations under the assumptions of isotropic elasticity. Equations of state of the host and the inclusion can be loaded as files created by other software in the EosFit7 program suite, or imported directly from thermodynamic databases such as Thermocalc. The complete range of EoS types supported by EosFit-7 are available in EosFit-Pinc. Fluid EoS can be provided in the form of PVT tables, which allows fluid inclusions to be modelled. Once loaded, the EoS of the host and inclusion can be used to calculate the entrapment isomeke from the measured remnant pressure of the inclusion. Or the final pressure can be calculated if the entrapment conditions are known or estimated. Calculations of the isochors of both the host and inclusion phases, and their mutual isomekes, can be performed, and output is provided in a format suitable for external plotting programs. The program EosFit-Pinc and the EosFit7 program suite are available at www.rossangel.net

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