

Combined thermal and FTIR analysis of porous silicon based nano-energetic films.

A. Plummer¹, V. A. Kuznetsov^{1, 2}, J. Gascooke¹, J. Shapter^{1, 3}, and N.H. Voelcker*⁴

¹*Centre of Expertise in Energetic Materials, School of Chemical and Physical Sciences, Flinders University, 5042, Bedford Park, Australia*

²*Weapons and Combat Systems Division, Defence Science and Technology Group, Edinburgh SA 5111, Australia*

³*Centre for Nanoscale Science and Technology, School of Chemical and Physical Sciences, Flinders University, 5042, Bedford Park, Australia*

⁴*Future Industries Institute, University of South Australia, 5095, Mawson Lakes, Australia*

*Corresponding Author: Prof. Nicolas H. Voelcker, Tel.: +61 8 8302 5508, email: nico.voelcker@unisa.edu.au.

Background correction of FTIR spectra

FTIR spectra of pSi samples heated continuously on a Linkam FTIR600 hot stage accessory heated at rate of 20 °C min⁻¹ were recorded on a Nicolet Nexus 870 FTIR using a liquid N₂ cooled MCT detector and 16 scans per measurement point.

Transmission spectra were collected at 1 minute intervals, between 30 and 510 °C at intervals of ≈ 20 °C. The raw interferograms for each spectrum were simultaneously recorded.

It is known that the IR transmission of crystalline Si decreases with increasing temperature due to increases in lattice vibrations within the crystal structure [1].

Accordingly, background spectra of a Si wafer were collected at the same temperature intervals as the sample temperatures (within 2 °C) – Figure S1 displays a selection of elevated temperature background spectra indicating the decrease in transmission across the entire spectral range under investigation. All raw data from individual experimental

samples were then recalculated to yield a sample spectrum corrected for the decreased Si wafer transmission at the corresponding temperature.

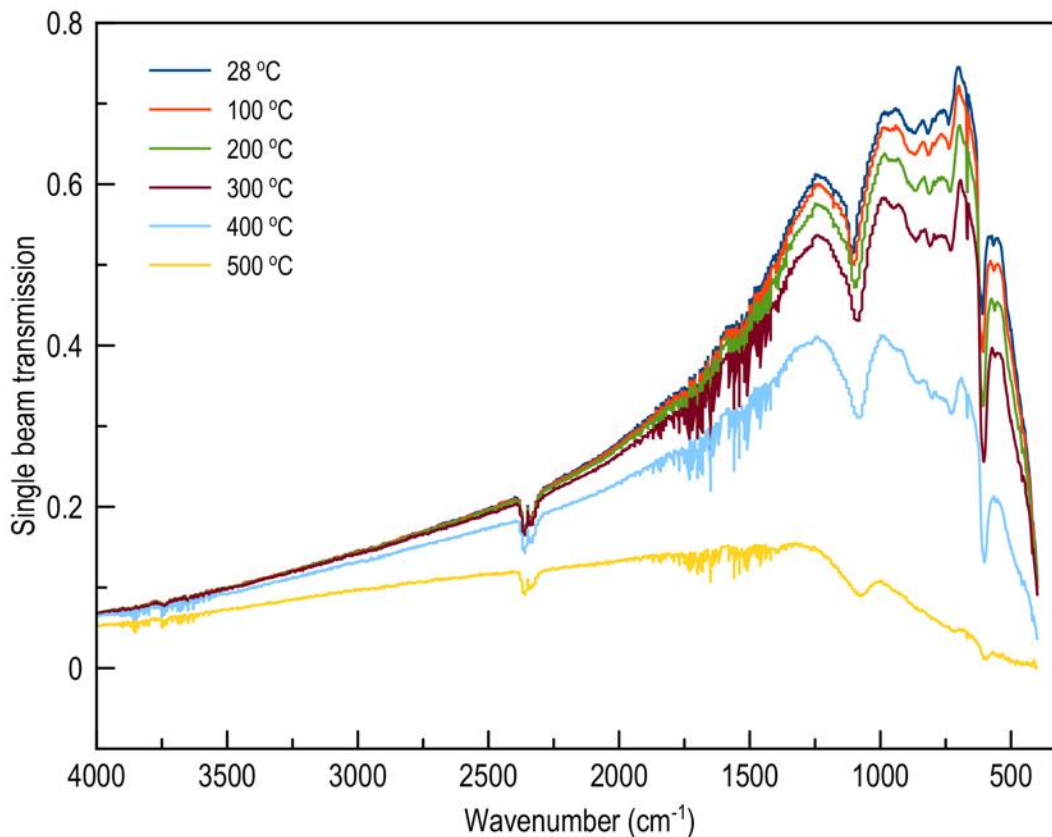


Figure S1: Single beam background transmission of unetched Si wafer at elevated temperatures.

Direct comparison of DSC to 1D and 2D FTIR data.

For each of the eight sample conditions investigated during this study, the DSC data have been aligned to the 2D FTIR scans, with selected 1D FTIR scans extracted below and above relevant transition temperatures, resented in Figures S2a to S2h.

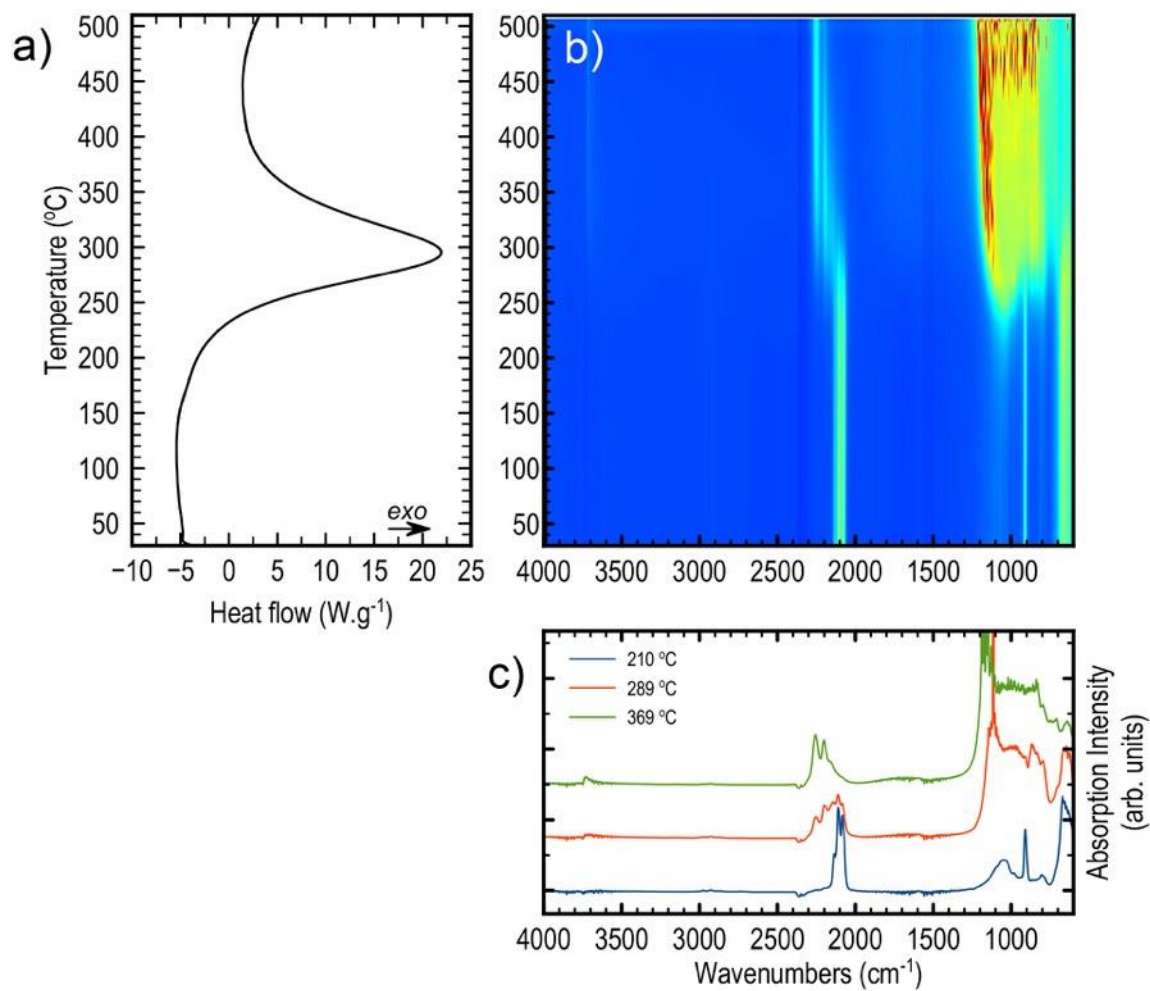


Figure S2a: Comparison of DSC scan (Panel a) to 2D FTIR spectrum (Panel b) for blank pSi in air. Selected 1D FTIR at temperatures below, equal to, and above relevant transition temperatures are presented in Panel c.

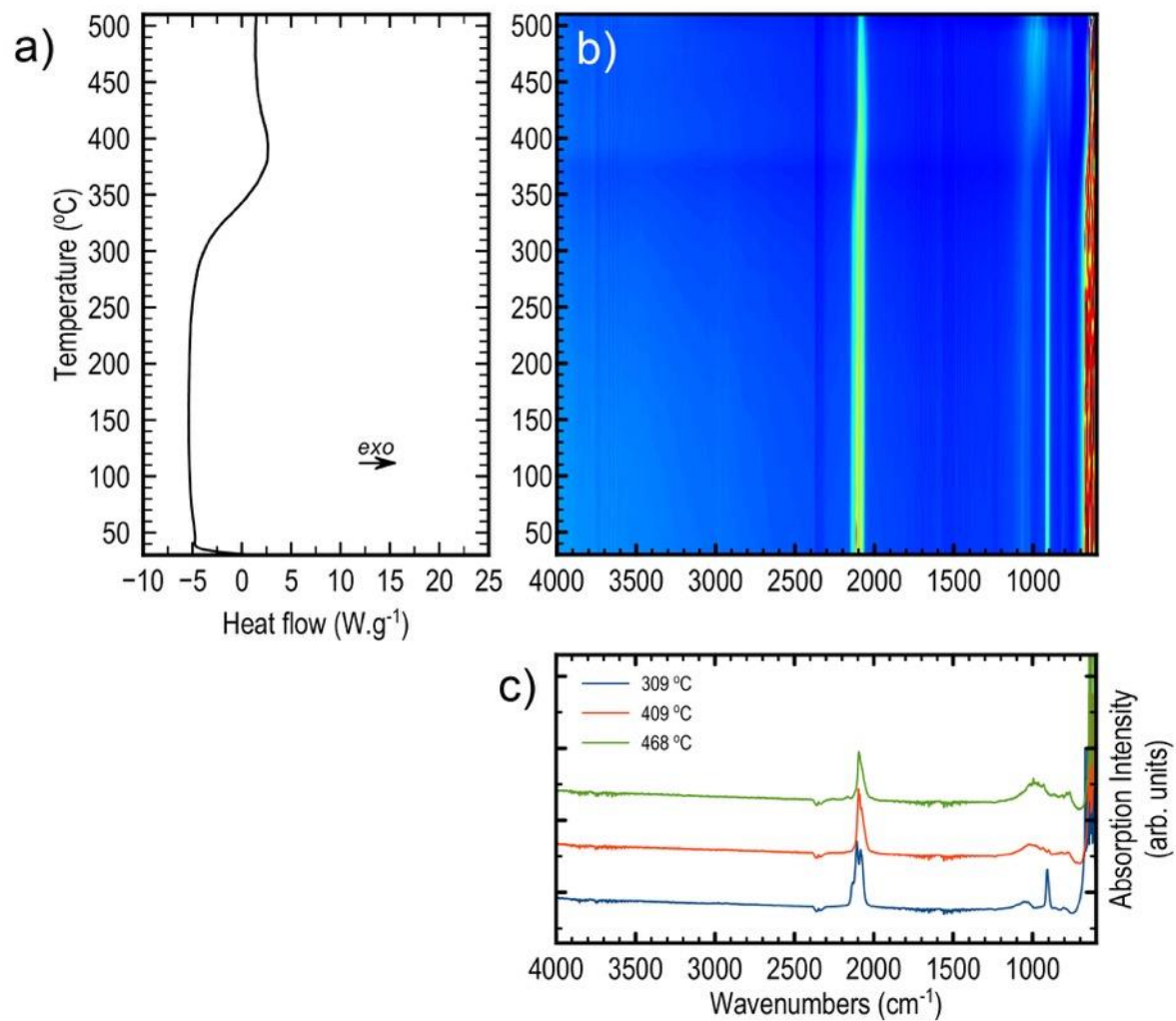


Figure S2b: Comparison of DSC scan (Panel a) to 2D FTIR spectrum (Panel b) for blank pSi in N₂. Selected 1D FTIR at temperatures below, equal to, and above relevant transition temperatures are presented in Panel c.

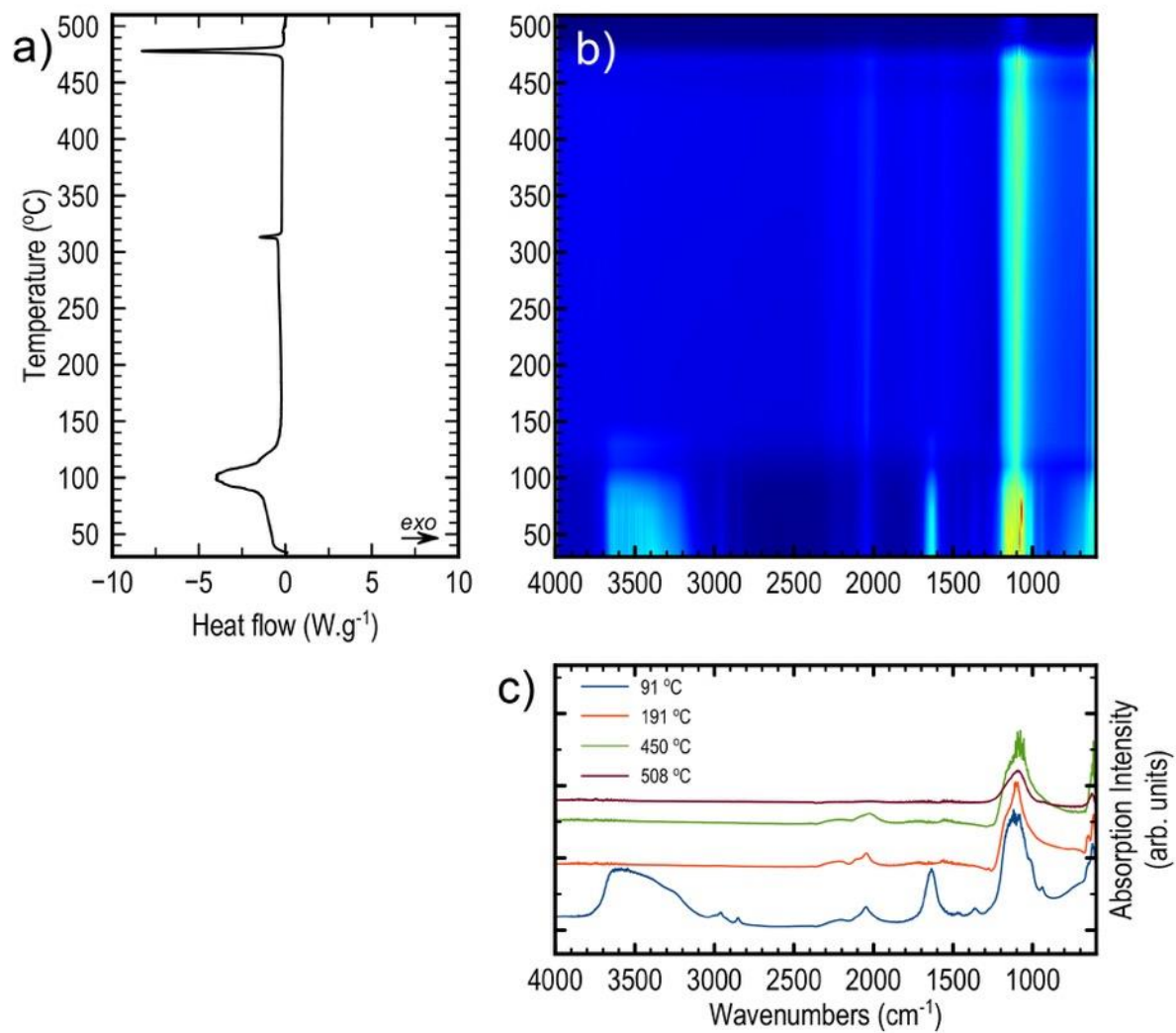


Figure S2c: Comparison of DSC scan (Panel a) to 2D FTIR spectrum (Panel b) for blank sodium perchlorate (SP) in N_2 . Selected 1D FTIR at temperatures below and above relevant transition temperatures are presented in Panel c.

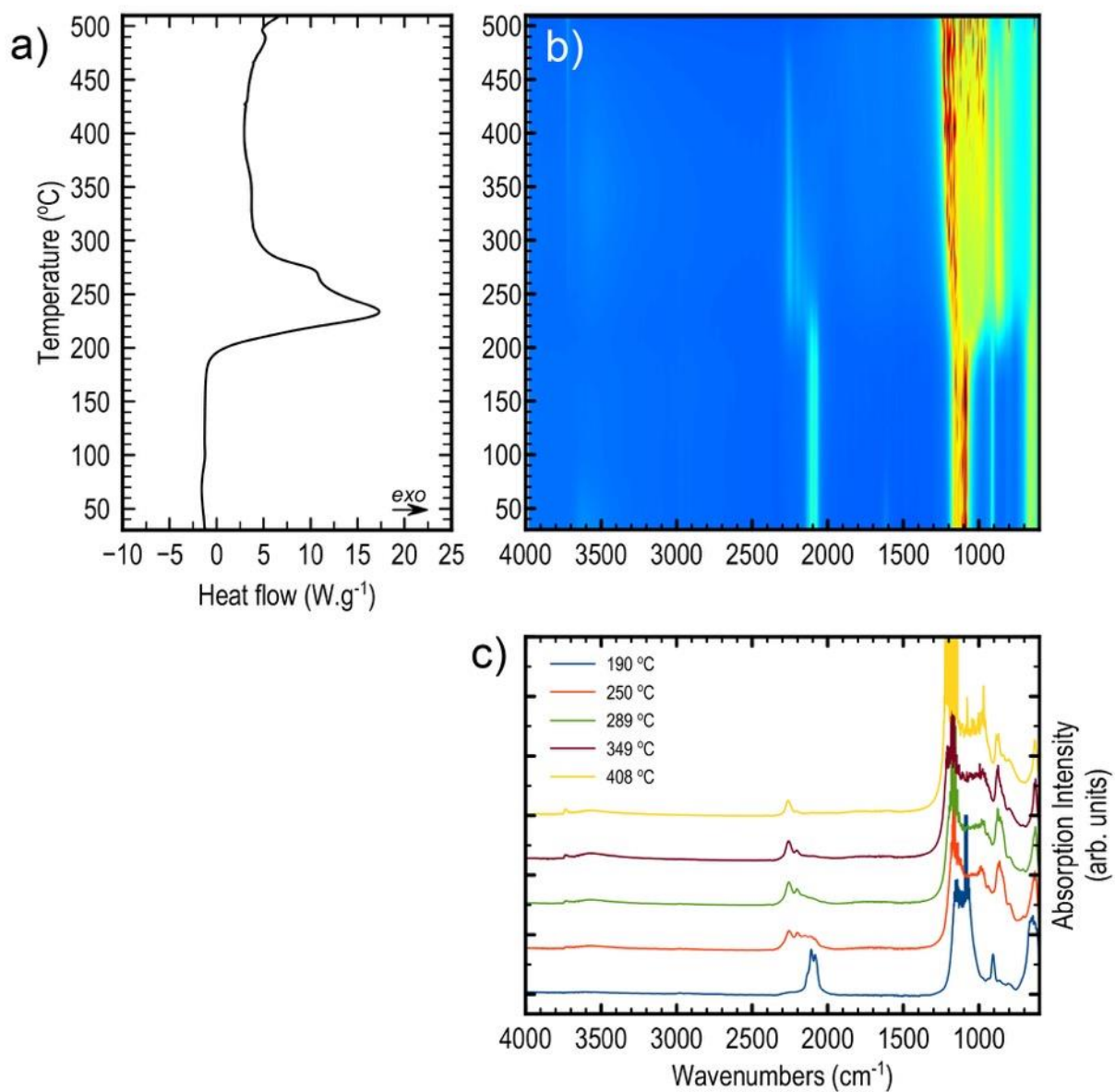


Figure S2d: Comparison of DSC scan (Panel a) to 2D FTIR spectrum (Panel b) for energetic pSi / SP mixture in air. Selected 1D FTIR at temperatures below, equal to, and above relevant transition temperatures are presented in Panel c.

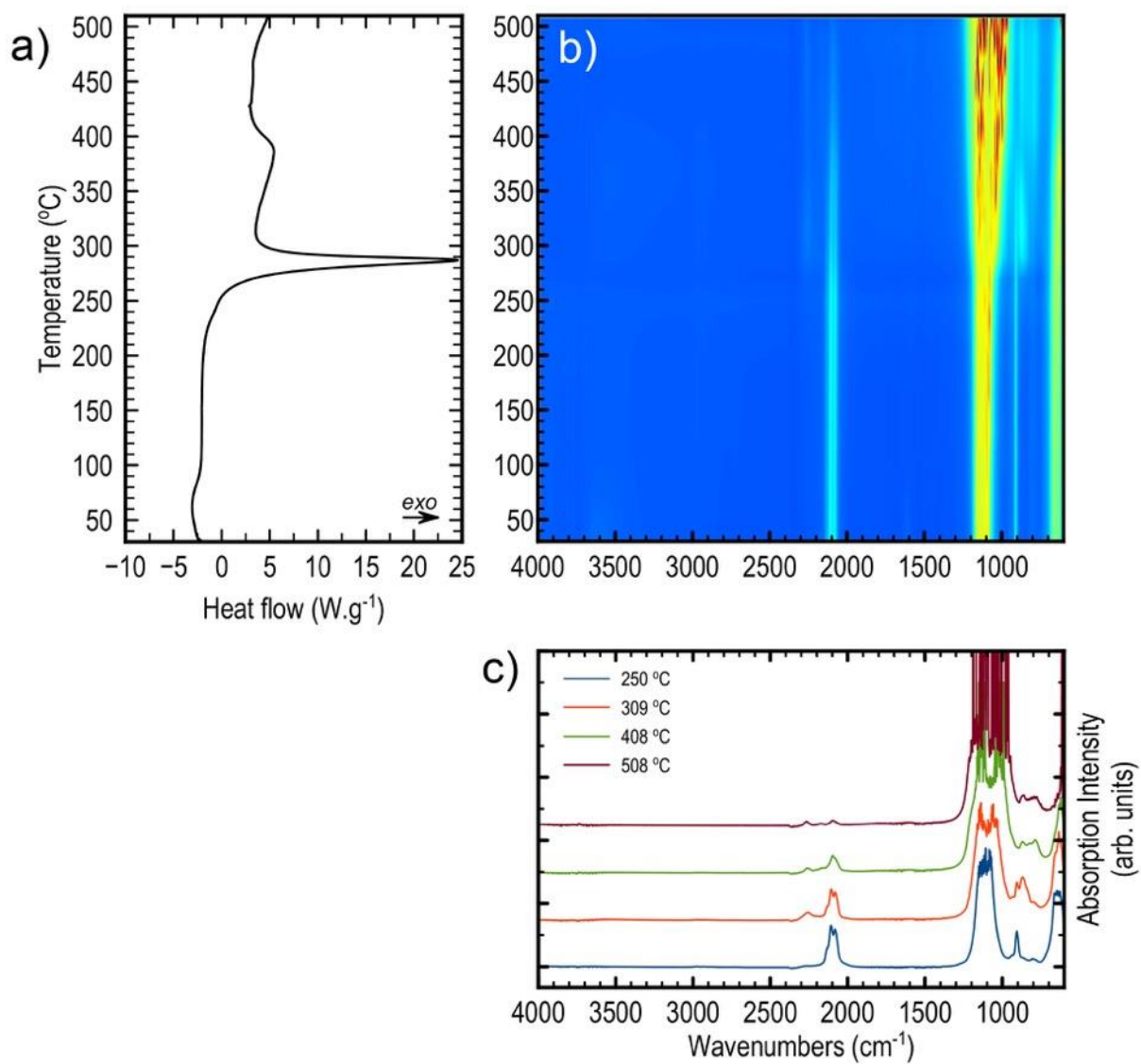


Figure S2e: Comparison of DSC scan (Panel a) to 2D FTIR spectrum (Panel b) for energetic pSi / SP mixture in N₂. Selected 1D FTIR at temperatures below, equal to, and above relevant transition temperatures are presented in Panel c.

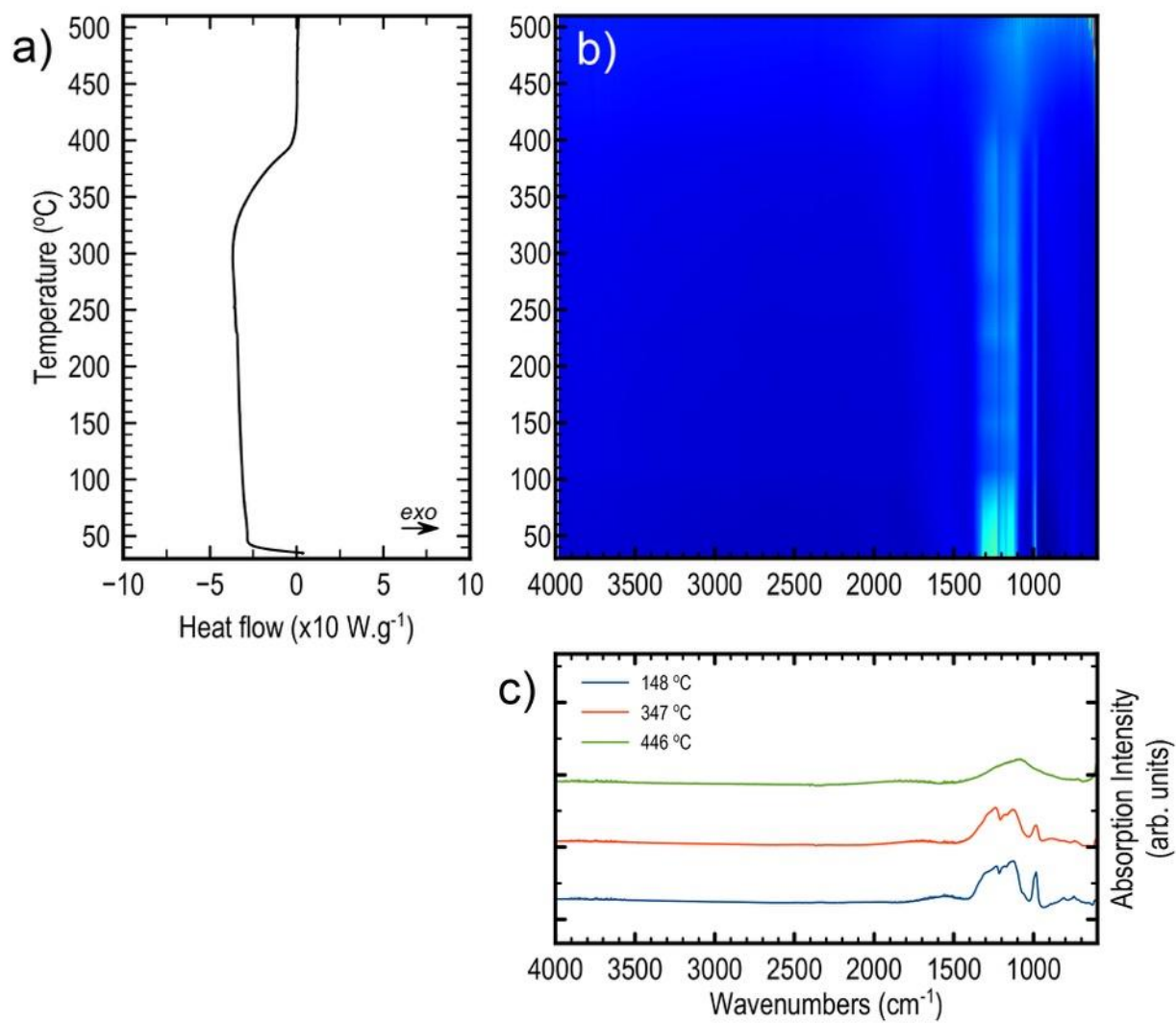


Figure S2f: Comparison of DSC scan (Panel a) to 2D FTIR spectrum (Panel b) for blank perfluoropolyether (PFPE) in N_2 . Selected 1D FTIR at temperatures below, equal to, and above relevant transition temperatures are presented in Panel c.

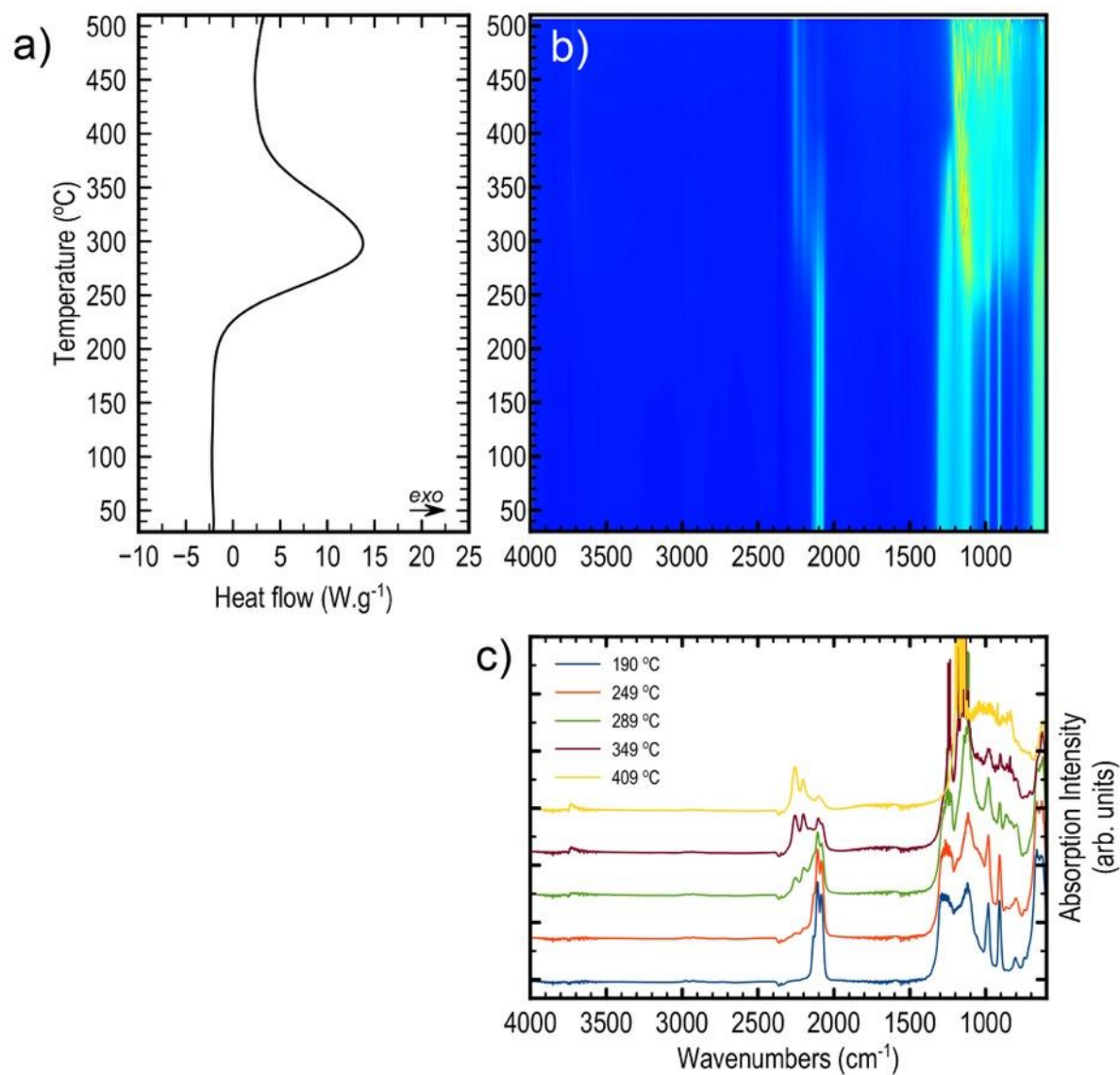


Figure S2g: Comparison of DSC scan (Panel a) to 2D FTIR spectrum (Panel b) for energetic pSi / PFPE mixture in air. Selected 1D FTIR at temperatures below, equal to, and above relevant transition temperatures are presented in Panel c.

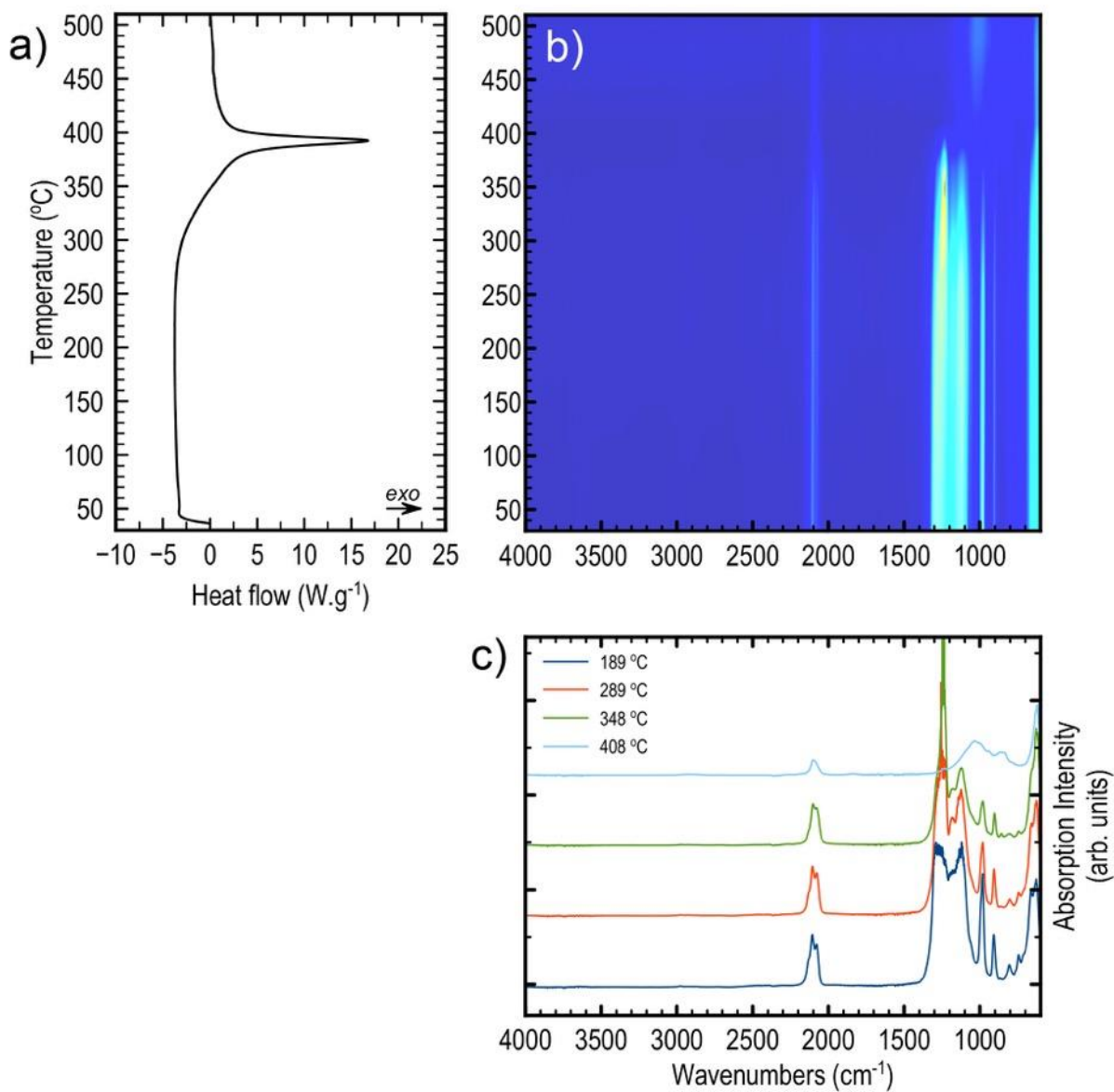


Figure S2h: Comparison of DSC scan (Panel a) to 2D FTIR spectrum (Panel b) for energetic pSi / PFPE mixture in N₂. Selected 1D FTIR at temperatures below, equal to, and above relevant transition temperatures are presented in Panel c.

Bibliography.

1. Boyd, I.W., T.D. Binnie, J.I.B. Wilsomn, and M.J. Colles, *Absorption of infrared radiation in silicon*. Journal of Applied Physics, 1983. **55**(8): p. 3.