

Electronic Supplement

The P-V-T equation of state of D₂O ice VI determined by neutron powder diffraction in the range $0 < P < 2.6$ GPa, $120 < T < 330$ K, and the isothermal equation of state of D₂O ice VII from 2 to 7 GPa at room temperature.

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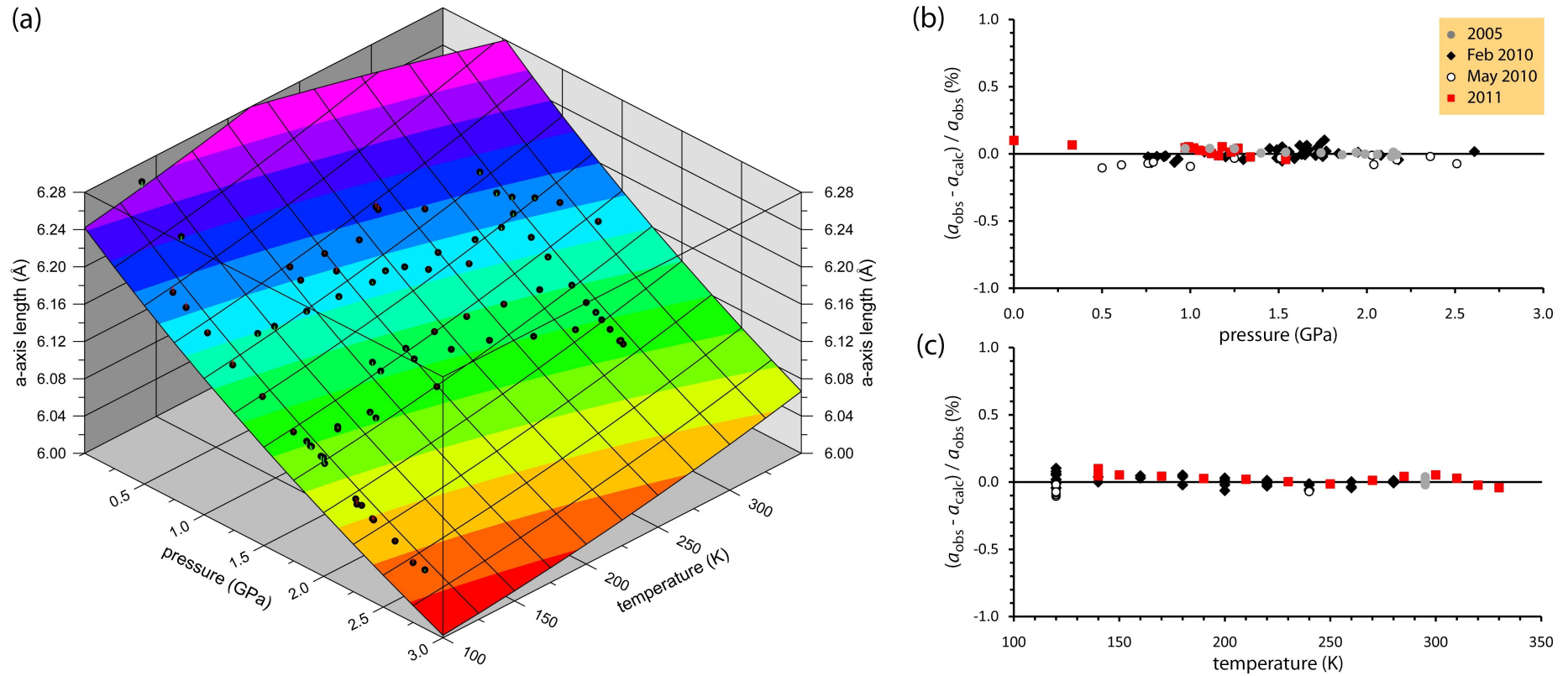
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This Electronic Supplement provides additional figures referred to in the main text of the paper.

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Figure S1

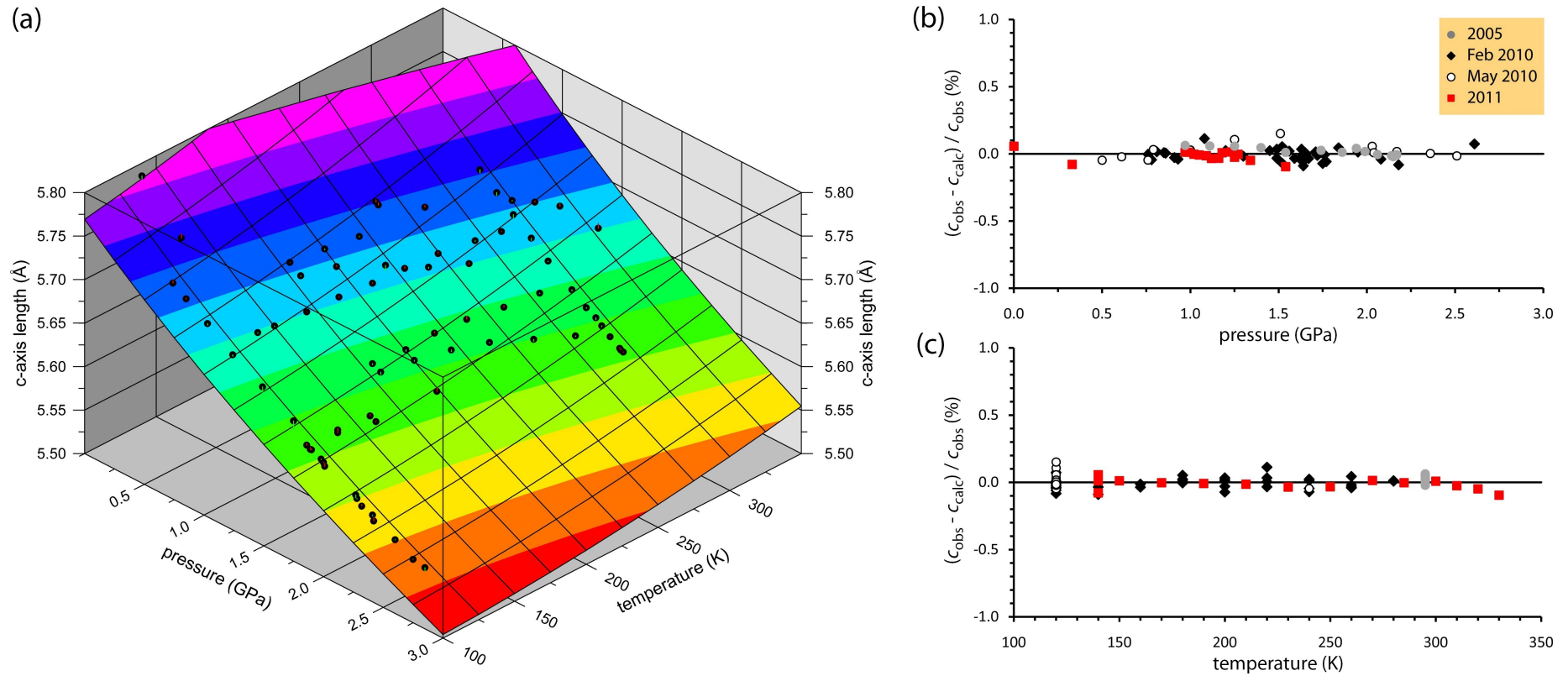
(a) Perspective view of the fitted P,T dependence of the *a*-axis of deuterated ice VI; data points are shown as filled circles, red tick marks attached to the data symbols indicate negative misfits and green tick marks indicate positive misfits. Surface contours are in increments of 0.02 Å. Parts (b) and (c) report the relative residuals as a function of pressure and temperature, respectively, the symbols corresponding to the four sample loadings.



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Figure S2

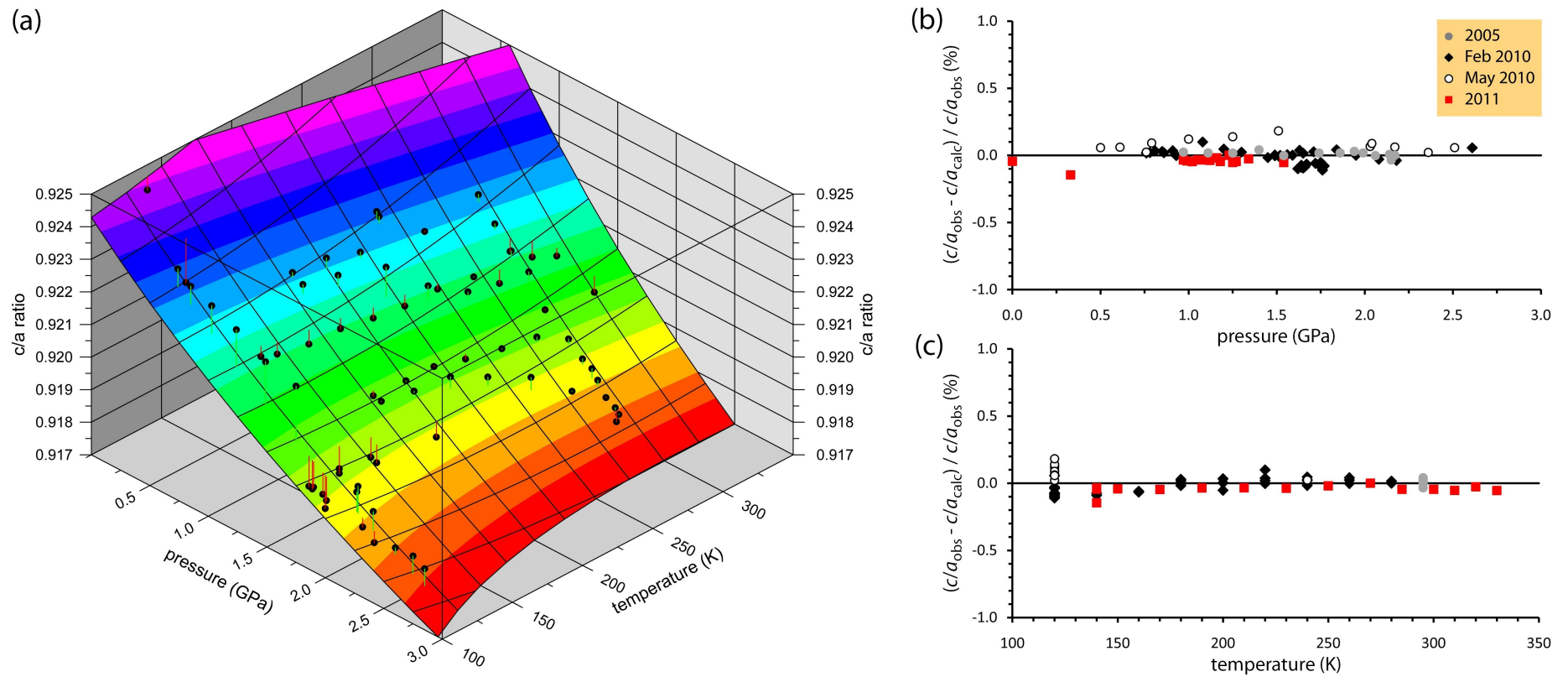
(a) Perspective view of the fitted P,T dependence of the *c*-axis of deuterated ice VI; data points are shown as filled circles, red tick marks attached to the data symbols indicate negative misfits and green tick marks indicate positive misfits. Surface contours are in increments of 0.025 Å. Parts (b) and (c) report the relative residuals as a function of pressure and temperature, respectively, the symbols corresponding to the four sample loadings.



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Figure S3

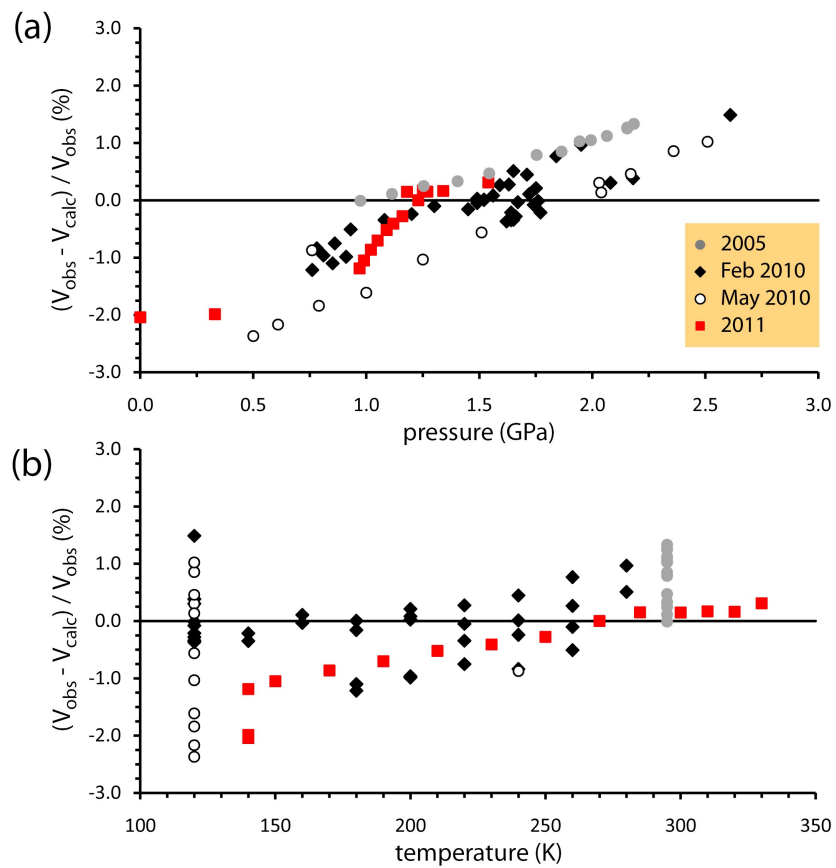
(a) Perspective view of the P,T dependence of the c/a axial ratio of deuterated ice VI computed from the P,T fits shown in Figures S2 and S3; data points are shown as filled circles, red tick marks attached to the data symbols indicate negative misfits and green tick marks indicate positive misfits. Surface contours are in increments of 0.0005. Parts (b) and (c) report the relative residuals as a function of pressure and temperature, respectively, the symbols corresponding to the four sample loadings.



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Figure S4

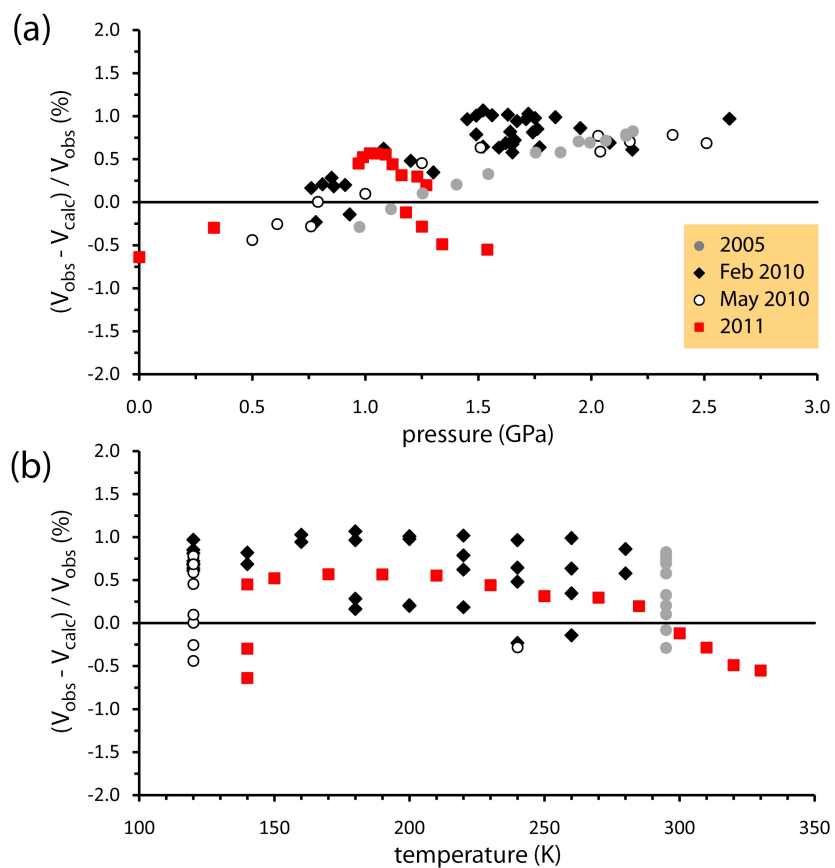
Deviation of our observed unit-cell volumes (symbols correspond to those used in Figure 1) from those predicted by the empirically-derived equation of state of Chizhov (1993), as a function of (a) pressure (for all temperature values) and (b) temperature (for all pressure values).



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Figure S5

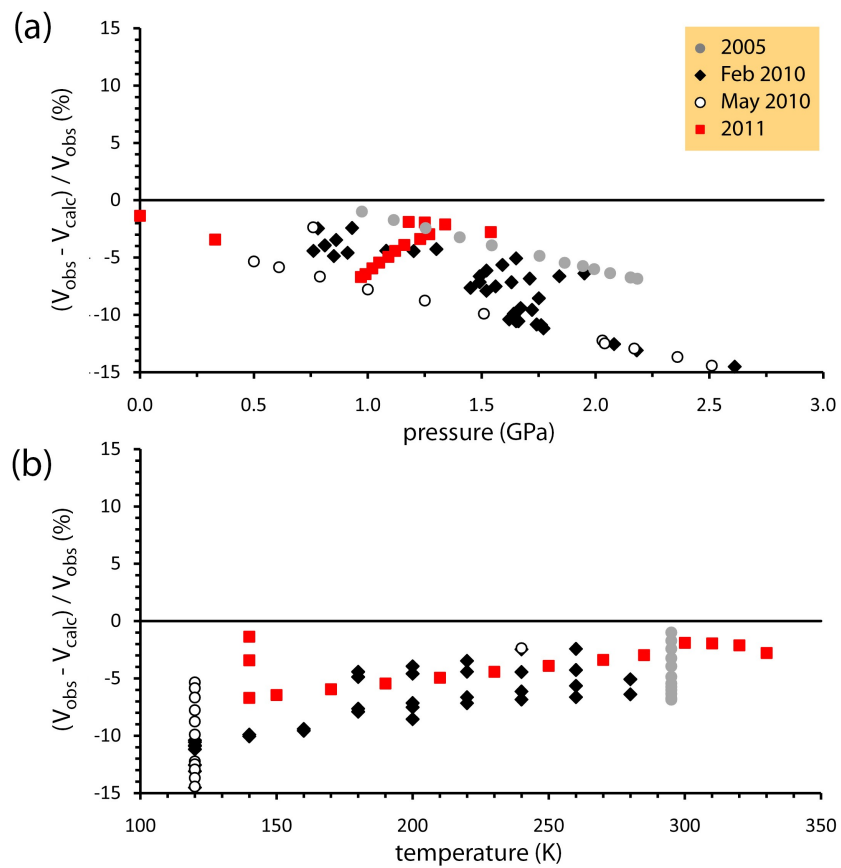
Deviation of our observed unit-cell volumes (symbols correspond to those used in Figure 1) from the empirically-derived equation of state of Fortes (2004), as a function of (a) pressure (for all temperature values) and (b) temperature (for all pressure values).



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Figure S6

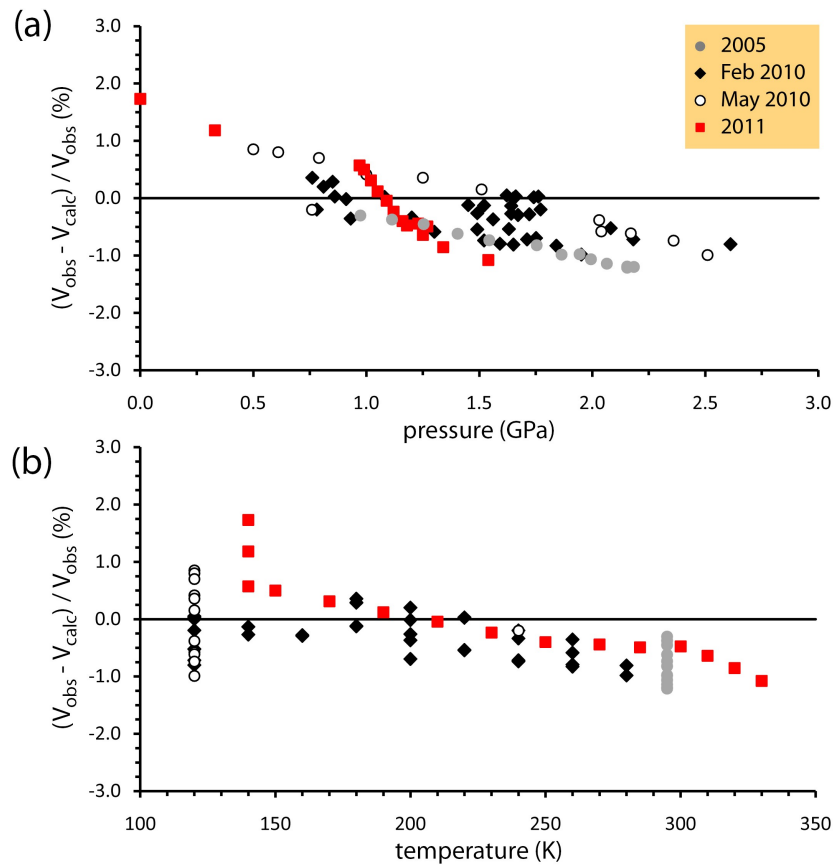
Deviation of our observed unit-cell volumes (symbols correspond to those used in Figure 1) from the empirically-derived equation of state of Choukroun & Grasset (2007), as a function of (a) pressure (for all temperature values) and (b) temperature (for all pressure values). Note the large difference in the vertical scale compared with Figures 7, 8 and 10.



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Figure S7

Deviation of our observed unit-cell volumes (symbols correspond to those used in Figure 1) from the computationally-derived equation of state of Noya *et al.* (2007), as a function of (a) pressure (for all temperature values) and (b) temperature (for all pressure values).



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References

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(doi:10.1021/jp0743121).

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