

Supplementary Information for:**Electronic transitions of iron in almandine-composition glass to 91 GPa**

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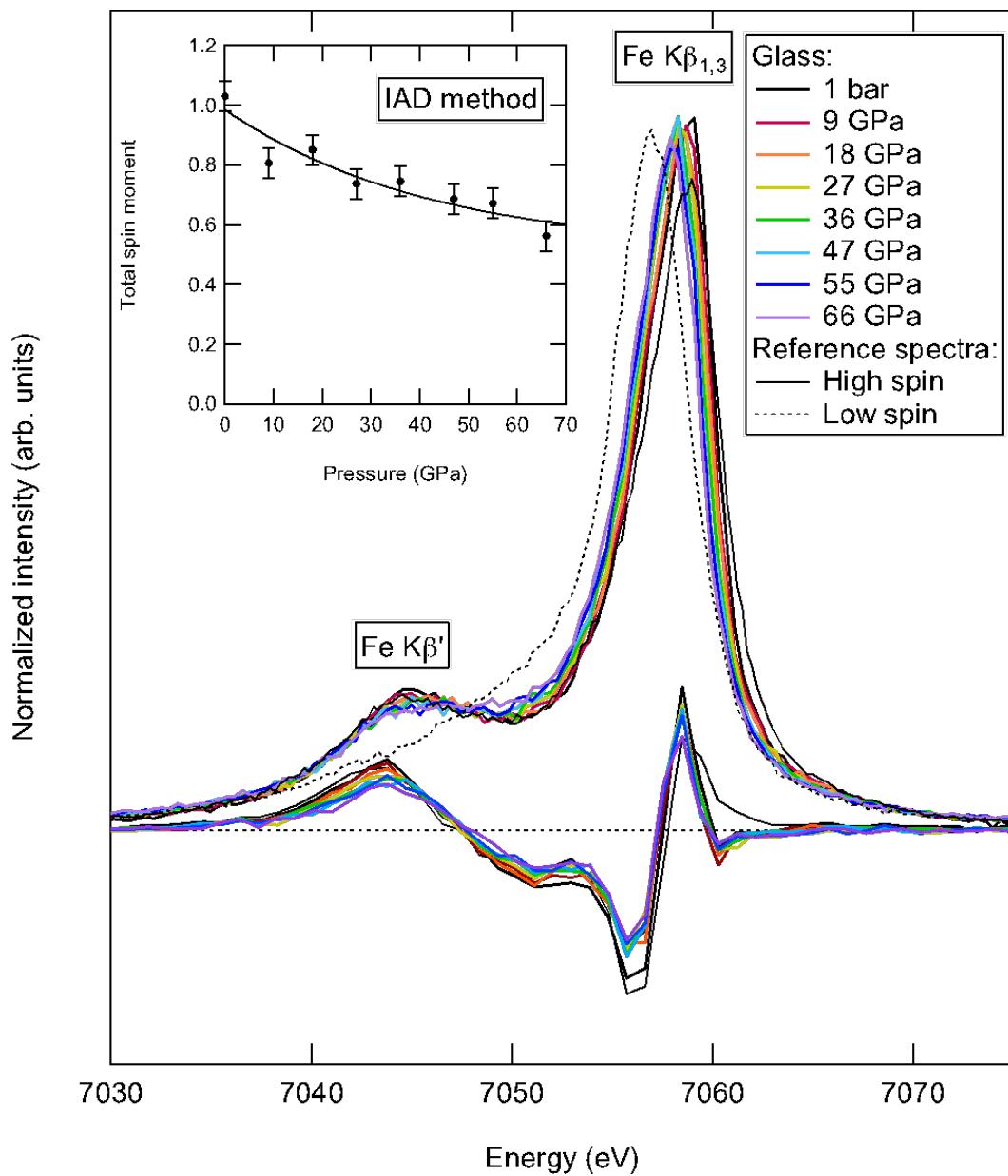
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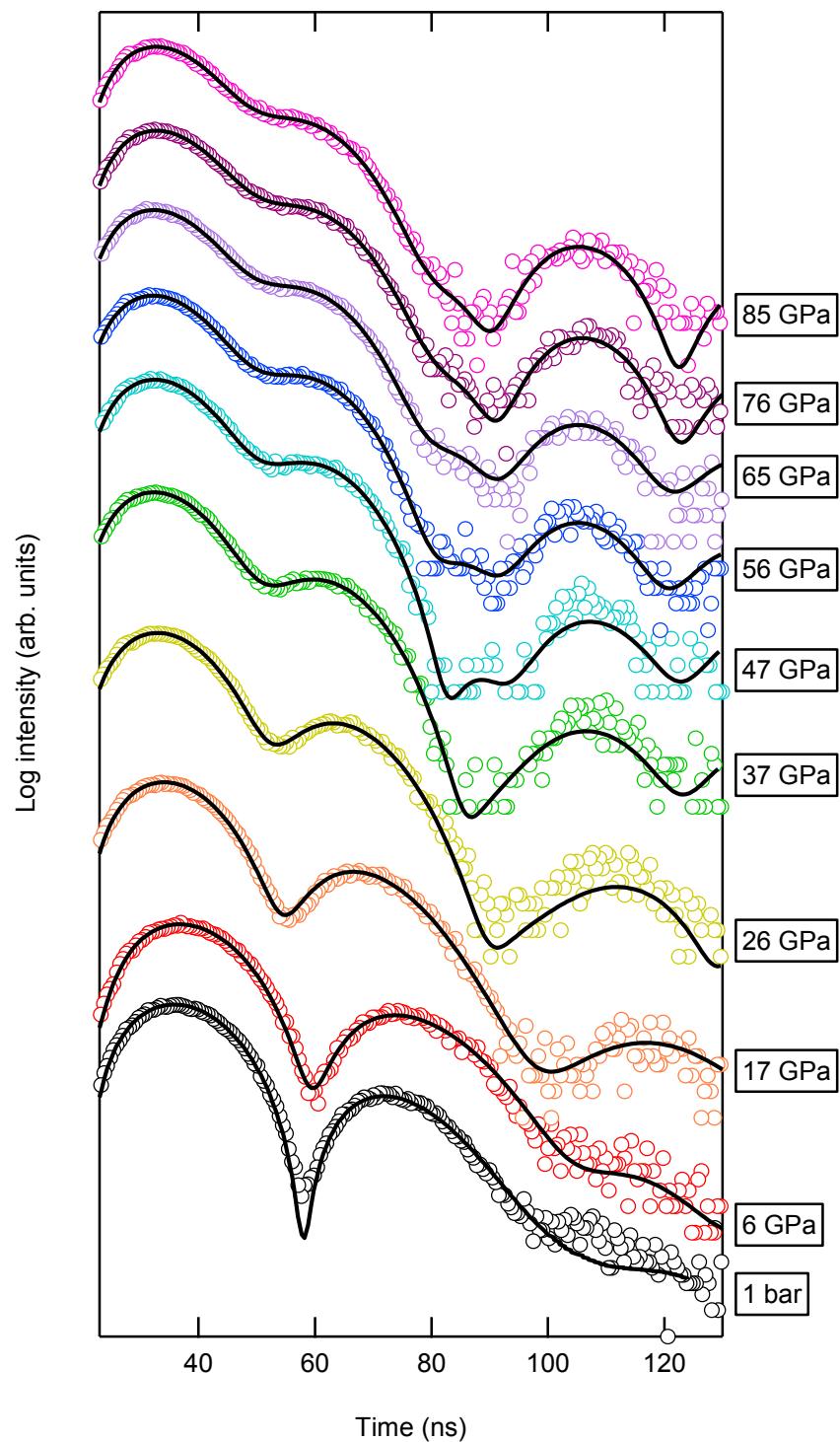
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Supplementary Table 1 : Composition of synthetic almandine glass determined by electron microprobe. All iron is reported as FeO.

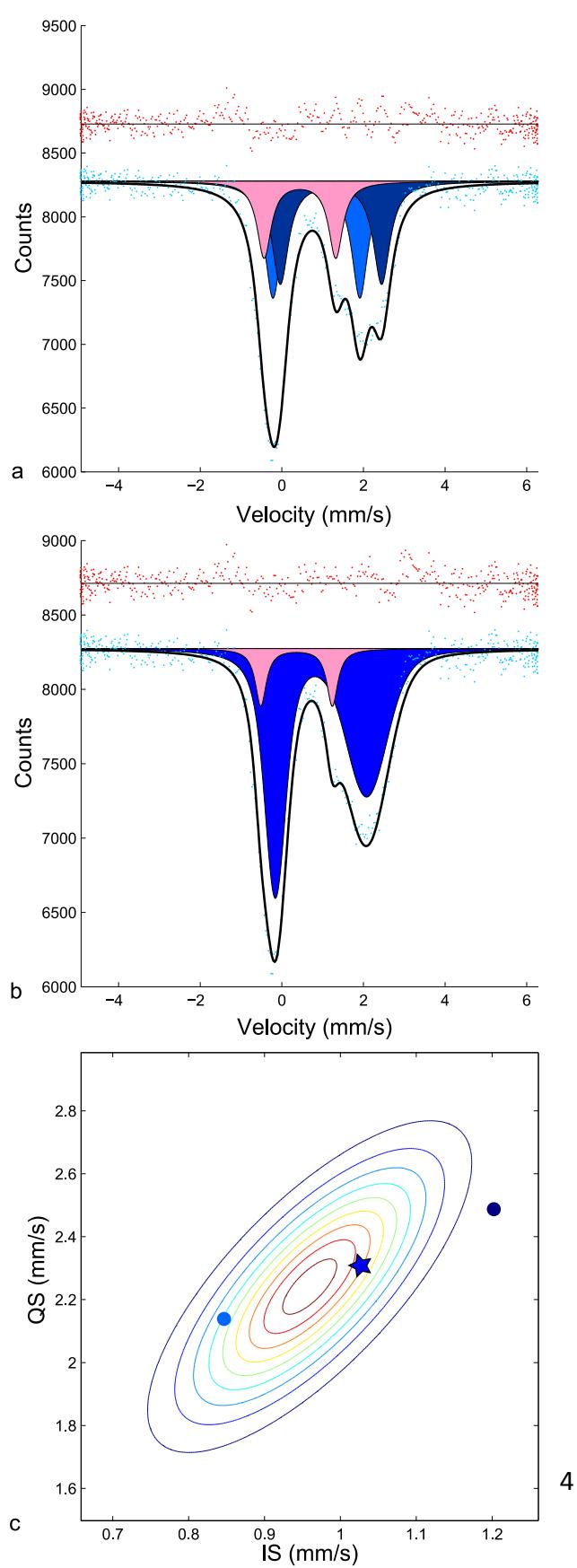
Oxide	Weight %	Formula cations
SiO ₂	35.73	2.99
TiO ₂	0.01	0.00
Al ₂ O ₃	22.06	2.18
Cr ₂ O ₃	0.02	0.00
FeO	39.10	2.74
MnO	0.00	0.00
MgO	0.01	0.00
CaO	0.01	0.00
Na ₂ O	0.06	0.01
Total	96.99	7.92



Supplementary Figure 1: Stacked XES spectra for almandine glass normalized to area and shifted to common center of mass (Vankó et al. 2006). Difference spectra below are relative to the low-spin (Mg,Fe)O reference (Lin et al. 2010). Inset: total spin moment calculated from integrated absolute difference between spectra and high- and low-spin (Mg,Fe)O references (Lin et al. 2010).



Supplementary Figure 2: Time-domain synchrotron Mössbauer spectra of almandine glass from 6–85 GPa. Fits to data are shown in black solid lines.



Supplementary Figure 3: Fits to energy-domain Mössbauer spectra of almandine glass in neon medium at 41 GPa using a) 3 Lorentzian doublets and b) 1 Lorentzian doublet and 1 doublet with correlated distribution in both quadrupole splitting and center shift, the extended Voigt-based fitting (xVBF) model (Lagarec and Rancourt 1997; Prescher et al. 2012). Pink doublets represent Fe³⁺ component while blue doublets represent Fe²⁺. c) The correlated distributions of the xVBF model shown in a contour plot. The weighted average (star) of the pair of doublets (circles) from a) is close to the mean of the correlated distribution in b), though with systematically higher IS and QS. Relative to a), the fit in b) also gives a slightly lower total intensity of the Fe²⁺ component.

References

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