This journal is © the Owner Societies 2010

Electronic Supplementary Information

^{31}P solid-state NMR studies of the short range order in phosphorus-selenium glasses

A. Bytchkov, F. Fayon, D. Massiot, L. Hennet and D. L. Price

Conditions Extrêmes et Matériaux : Haute Température et Irradiation (CEMHTI), 1D Av. Recherche Scientifique, 45071 Orléans Cedex 2, France, and Université d'Orléans, Faculté des Sciences, Av. Parc Floral, 45067 Orléans Cedex 2, France

Content:

ESI Figure 1: Glass densities in the two glass-forming regions of the P-Se system.

ESI Figure 2: Measured glass transition temperatures of the P-Se system. The glass with 67 at.% of P showed two distinct T_g's, the lower one being similar to Se-rich glasses.

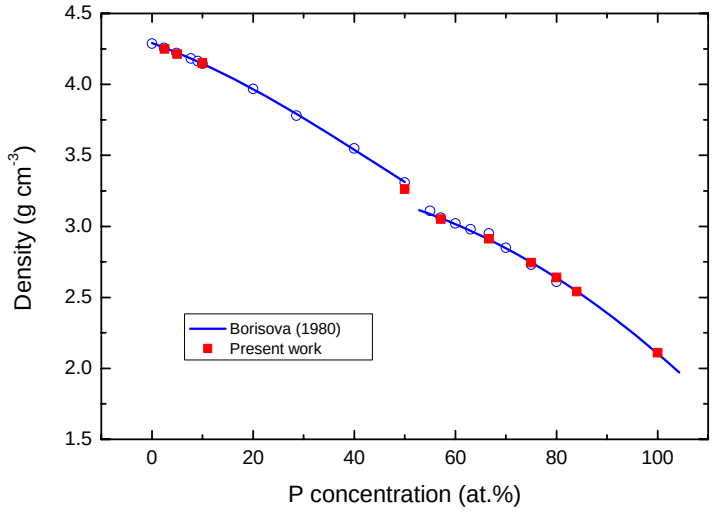
ESI figure 3: 2D DQ-SQ through-bond MAS correlation spectrum of crystalline α-P_4Se_3 recorded using the refocused INADEQUATE at a spinning frequency of 26 kHz with a DQ excitation and reconversion times of 0.96 ms. The projection along the SQ dimension (black) and conventional 1D MAS spectrum (blue) are shown above the 2D spectrum.

ESI figure 4: 2D DQ-SQ through-bond MAS correlation spectrum of crystalline β-P_4Se_3 recorded using the refocused INADEQUATE at a spinning frequency of 12 kHz with a DQ excitation/reconversion time of 2.0 ms. The projection along the SQ dimension is shown above the 2D spectrum.

ESI figure 5: Experimental (black) ^{31}P MAS spectra of Se-rich phosphorus selenium glasses and their best fits (dashed red) including spinning sidebands, with the resonances of $_{2/2}$SeP-P$Se_{2/2}$ (green), P_4Se_3 (violet), $P(Se_{1/2})_3$ (blue) and $Se{=}P(Se_{1/2})_3$ (grey) structural units.

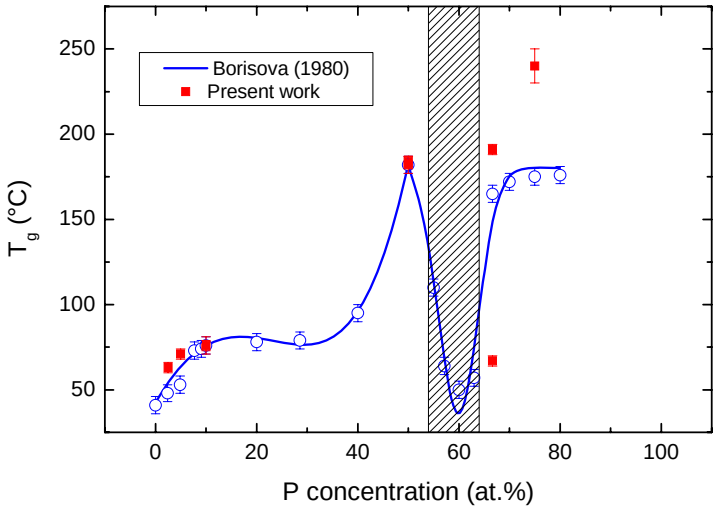
ESI figure 6: Experimental (black) ^{31}P MAS spectra of P-rich phosphorus selenium glasses and their best fits (dashed red) with the resonances assigned to of P_4Se_3 (violet), amorphous red-P like network and the two unidentified peaks.

This journal is © the Owner Societies 2010



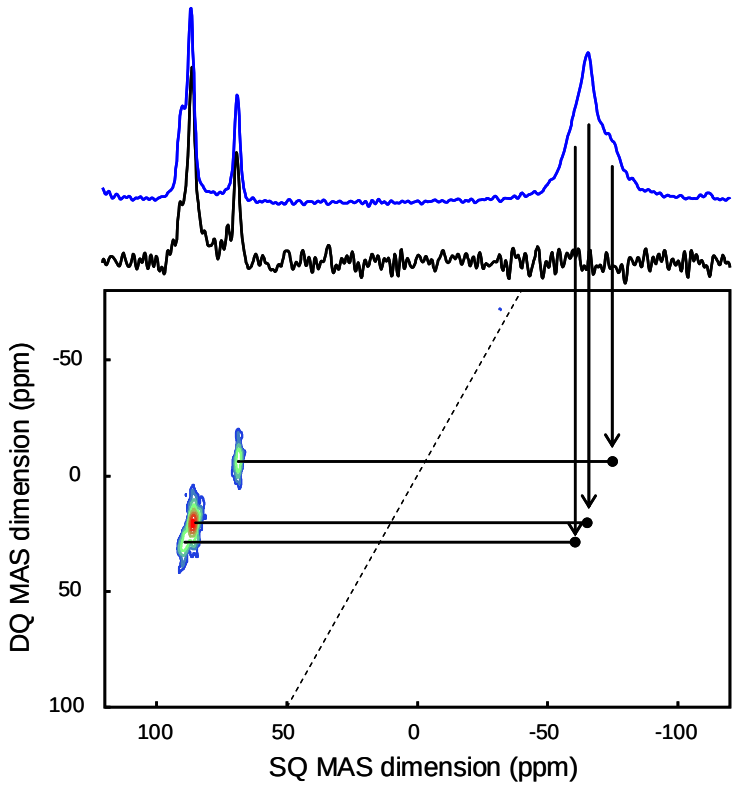
ESI Figure 1: Glass densities in the two glass-forming regions of the P-Se system.

This journal is © the Owner Societies 2010



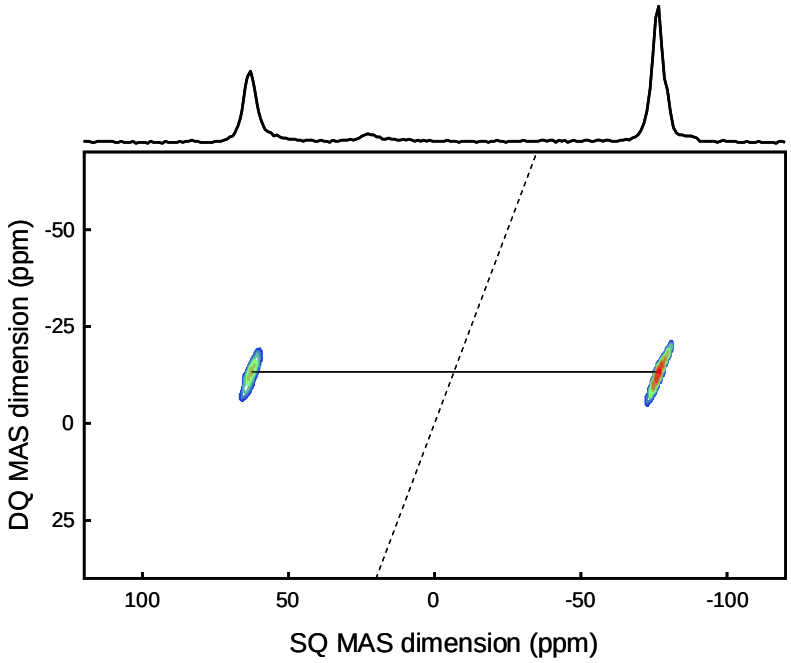
ESI Figure 2: Measured glass transition temperatures of the P-Se system. The glass with 67 at. % of P showed two distinct T_g's, the lower one being similar to Se-rich glasses.

This journal is © the Owner Societies 2010

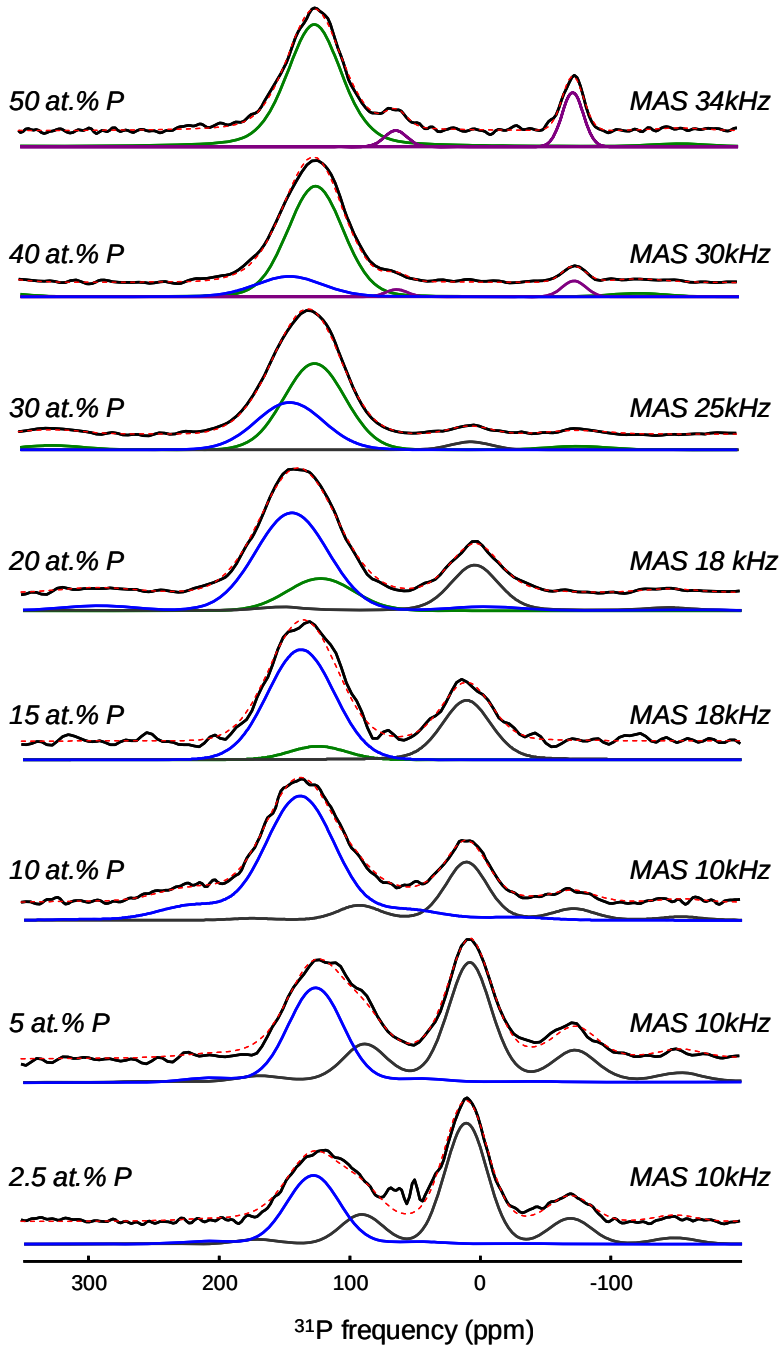


ESI figure 3: 2D DQ-SQ through-bond MAS correlation spectrum of crystalline α-P_4Se_3 recorded using the refocused INADEQUATE at a spinning frequency of 26 kHz with a DQ excitation and reconversion times of 0.96 ms. The projection along the SQ dimension (black) and conventional 1D MAS spectrum (blue) are shown above the 2D spectrum.

This journal is © the Owner Societies 2010



ESI figure 4: 2D DQ-SQ through-bond MAS correlation spectrum of crystalline β-P_4Se_3 recorded using the refocused INADEQUATE at a spinning frequency of 12 kHz with a DQ excitation/reconversion time of 2.0 ms. The projection along the SQ dimension is shown above the 2D spectrum.



ESI figure 5: Experimental (black) ^{31}P MAS spectra of Se-rich phosphorus selenium glasses and their best fits (dashed red) including spinning sidebands, with the resonances of $_{2/2}$SeP-PSe$_{2/2}$ (green), P_4Se_3 (violet), $P(Se_{1/2})_3$ (blue) and $Se{=}P(Se_{1/2})_3$ (grey) structural units.