

Electronic Supporting Information for the manuscript

Magnetic Structures of $Fe_{32+\delta}Ge_{33}As_2$ and $Fe_{32+\delta}Ge_{35-x}P_x$ Intermetallic Compounds: A Neutron Diffraction and ^{57}Fe Mössbauer Spectroscopy Study

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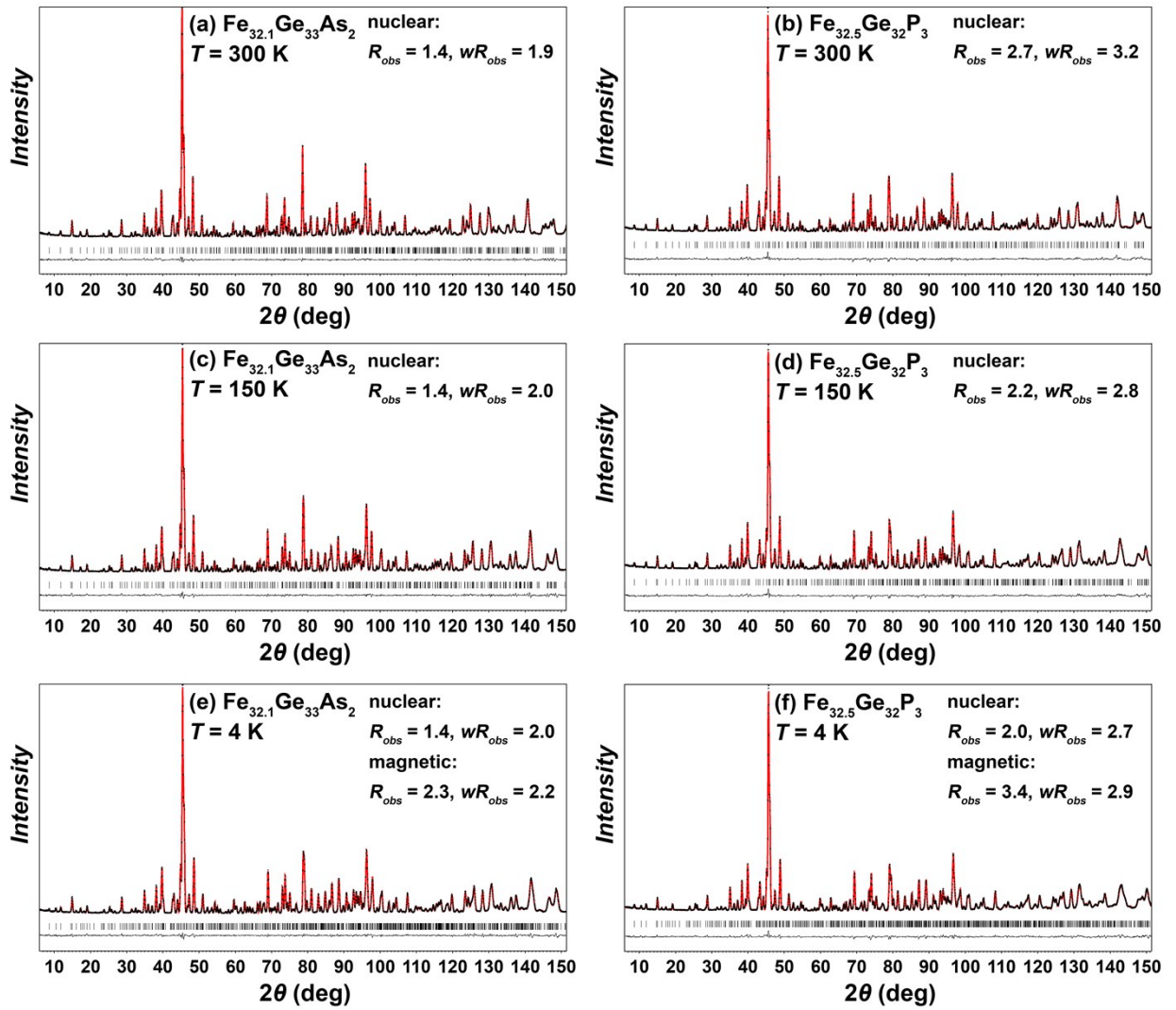


Fig. S1 Experimental (black points) and calculated (red line) high-resolution neutron powder diffraction patterns of $\text{Fe}_{32.1}\text{Ge}_{33}\text{As}_2$ (left) and $\text{Fe}_{32.5}\text{Ge}_{32}\text{P}_3$ (right) recorded on the SPODI diffractometer ($\lambda = 1.5482 \text{ \AA}$). Peak positions (black ticks) and the difference plot (black line) are given in the bottom part of each panel. The panels (a, b) refer to room temperature; (c, d) - to lower temperature above T_N ; (e, f) - to the low-temperature magnetic structure. Above T_N , the calculated patterns correspond to crystal structure refinements within the $P6/mmm$ space group, while the ones below T_N - to magnetic structure refinements within the P_b2_1/m magnetic space group.

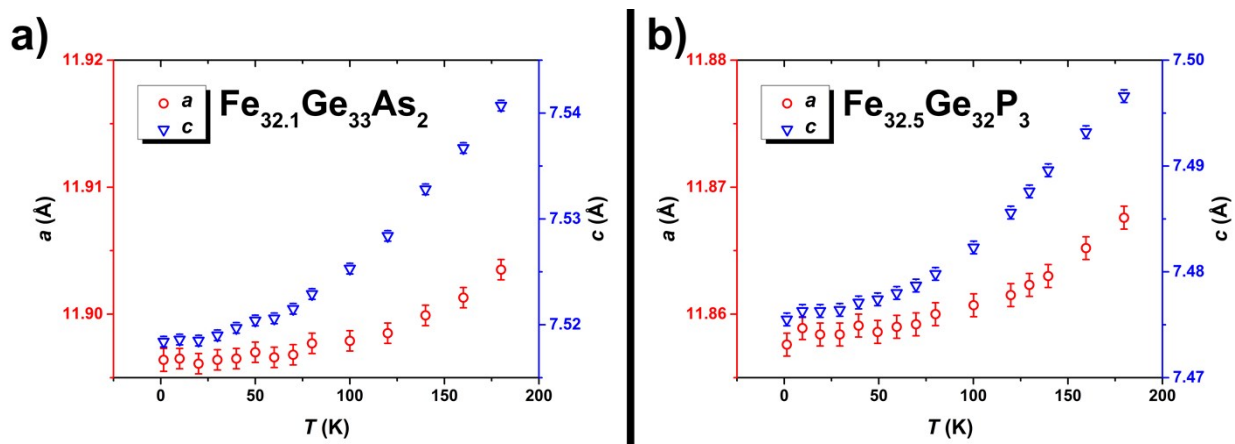


Fig. S2. The temperature dependence of the cell parameters from G4.1 neutron diffraction data for $\text{Fe}_{32.1}\text{Ge}_{33}\text{As}_2$ (a) and $\text{Fe}_{32.5}\text{Ge}_{32}\text{P}_3$ (b).

Table S1 Atomic charges estimated by electron density analysis from the DFT calculations.

Site	Charge
As1	-0.11
Ge1	-0.22
Ge2	-0.17
Ge3	-0.14
Ge4	-0.25
Ge5	-0.06
Fe1	+0.16
Fe2	+0.21
Fe3	+0.18
Fe4	+0.19

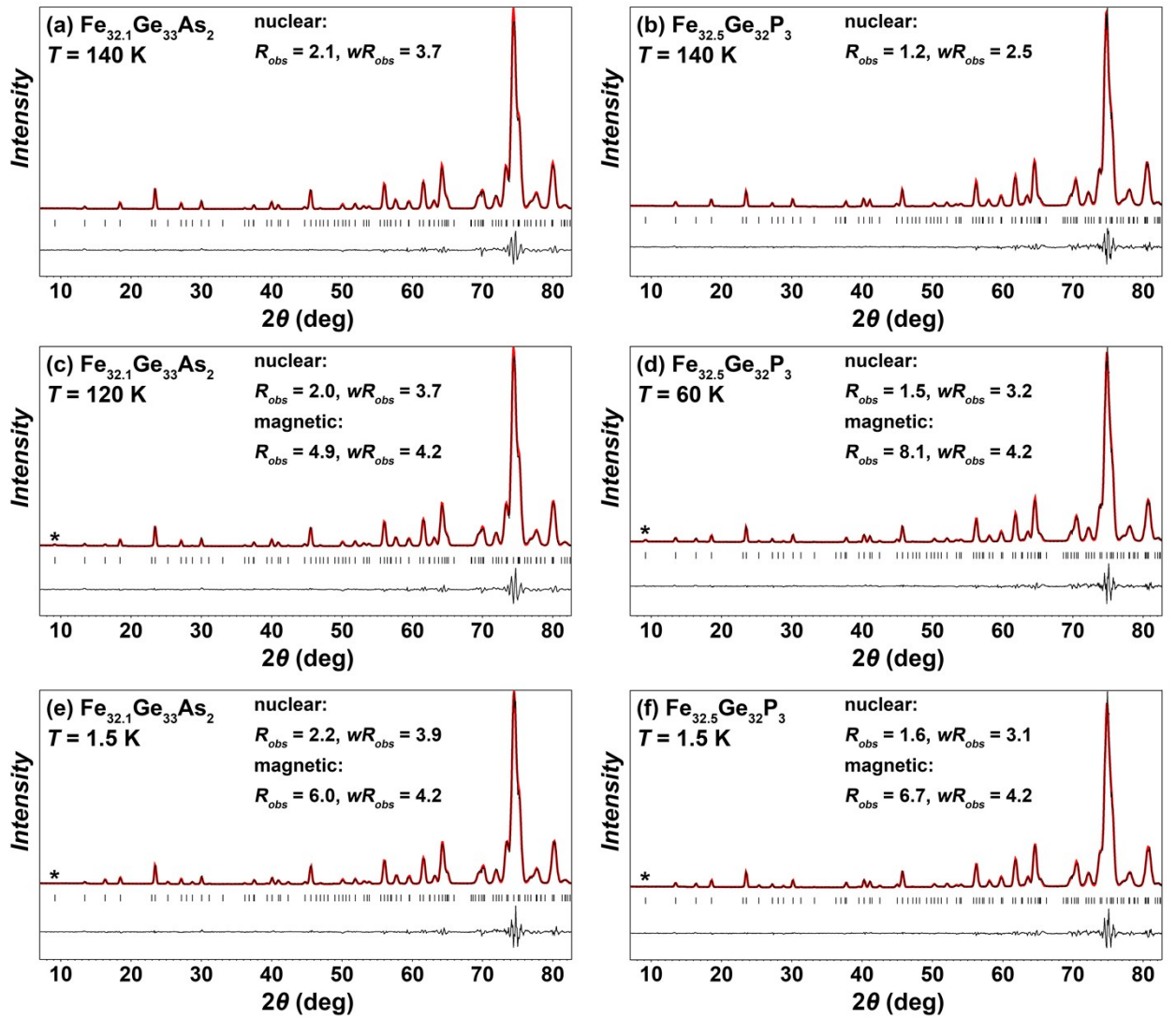


Fig. S3 Experimental (black points) and calculated (the P_b2_1/m magnetic space group, red line) low-angle neutron powder diffraction patterns of $\text{Fe}_{32.1}\text{Ge}_{33}\text{As}_2$ (left) and $\text{Fe}_{32.5}\text{Ge}_{32}\text{P}_3$ (right) recorded on the G4.1 diffractometer ($\lambda = 2.423 \text{ \AA}$). Peak positions (black ticks) and the difference plot (black line) are given in the bottom part of each panel. The panels (a, b) refer to the paramagnetic state; (c, d) – high-temperature regions, and (e, f) – low-temperature regions. The $(0; 0; 1/2)$ magnetic peak is marked by the asterisk.