Fig. 1 Experimental ^{77}Se ∂_{ii} values against the chemical shieldings components computed for experimental (left) and relaxed (right) cristalline structures. The line corresponds to the linear least-square fit of the corresponding data, the equation is presented on the graph.
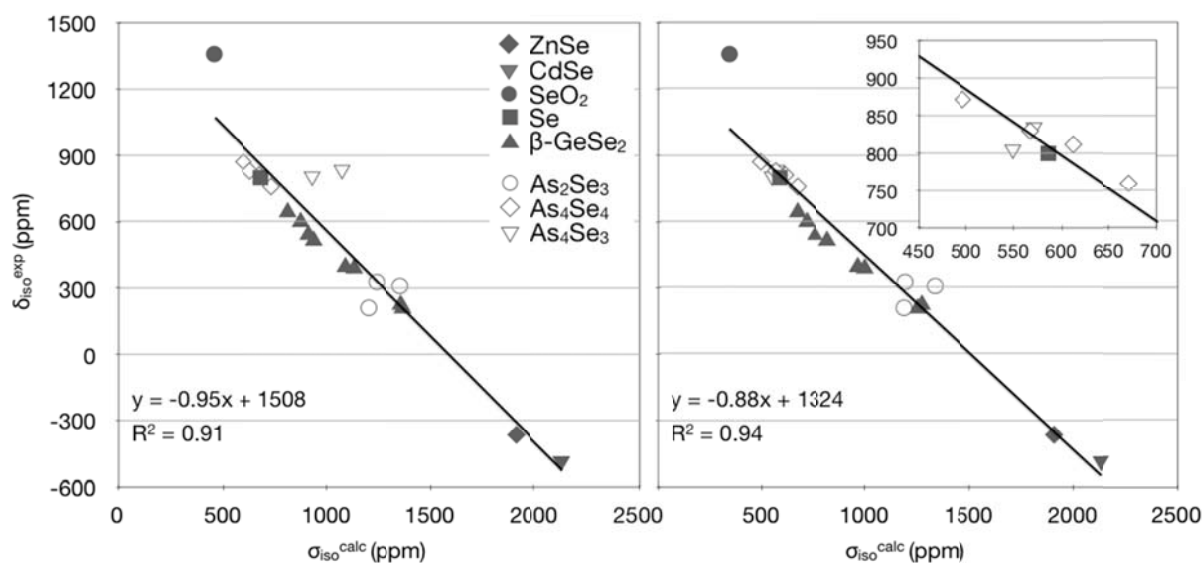

Fig. 2 Experimental ^{77}Se chemical shifts against the isotropic chemical shieldings computed for all experimental (left) and relaxed (right) cristalline structures. The line corresponds to the linear least-square fit of the corresponding data, the equation is presented on the graph.
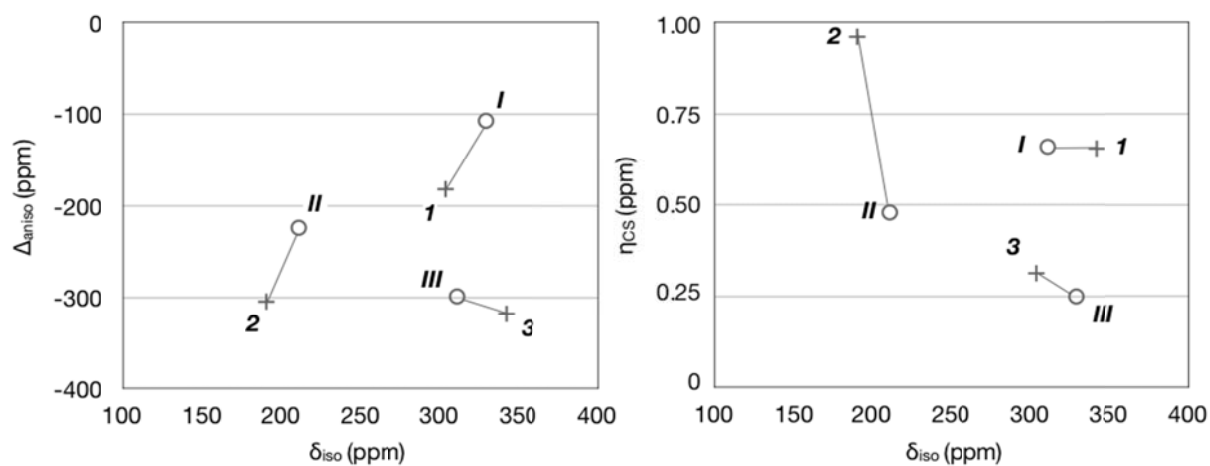
Fig. 3 Experimental (circles) and theoretical (plus) Δ_{aniso} (left) and η_{CS} (right) *vs* the corresponding isotropic chemical shifts for the crystalline structure of As_2Se_3.