SOUTENANCE DE THESE

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The highly fragile glass former Decalin

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Systems exhibiting the glass transition can be classified by fragility. In this work we studied structural and dynamical aspects of highly fragile C10 H18 Decalin. Trans Decalin is locked into a pseudo-flat centrosymmetric conformation, while cis Decalin interchanges dynamically between chiral, pseudo-spherical ground states. On investigation of the phase behaviour trans Decalin was found to crystallise rapidly and cleanly; its crystal structure could be determined. From the crystal structure the dynamics of crystalline trans Decalin could be calculated using ab-initio lattice energy calculations and compared to measurements. Using neutron diffraction and mol. dynamics simulations the amorphous structure of Decalin was investigated. The difference in structure to the common molecular liquid Cumene is significant. The features of the amorphous structure of sphere-like cis Decalin show strong resemblance to the ones of Argon and metallic glasses. The dynamics of Decalin were investigated in the slightly supercooled liquid range. Using neutron scattering and optical spectroscopy, data was collected for a wide spectral range and several temperatures. The data suggests high fragility for the generic Decalin mix, which is in agreement with reported results. By contrast to previous estimations, an extrapolation of our data indicates cis Decalin to be only slightly less fragile than the generic mixture. Finally a lower limit to the four point susceptibility function chi4 could be calculated and the number of correlated molecules determined. The evolution of this value as a function of Tg /T and relaxation time are in agreement with literature.