

Dynamics and orientation of parathion dissolved in a discotic nematic lyomesophase

Vera, Alejandra

Ahumada, Hernán

Bahamonde, Victor

Montecinos, Rodrigo

Araya-Maturana, Ramiro

Muñoz, Daniel

Weiss-López, Boris E.

Parathion, an organophosphorous pesticide, presents serious hazards to the environment and health. It inhibits acetylcholinesterase, an enzyme incorporated in the cell membrane. A study on the behaviour of parathion in a lipid environment is interesting from environmental cleaning and biological perspectives. ^2H NMR quadrupole splittings (Q) and longitudinal relaxation times (T1) of parathion- d_4 , dissolved in a nematic discotic lyomesophase made of tetradecyltrimethylammonium chloride/decanol (10% 1,1-dideuterodecanol)/water (0.1% D_2O)/NaCl, have been measured. Q and T1 from DHO and 1,1-dideuterodecanol were also obtained. For a detailed understanding of the experimental results, a 19 ns molecular dynamics (MD) simulation of a bilayer fragment including three parathion molecules was calculated. Parathion is strongly attached to the aggregate and the solubilization increases the alignment of the interface components. Calculated densities show that parathion is located in the hydrophobic