The samples of hydrotalcite intercalated with pyrenetetrasulphonate acid were obtained. Their structure cannot be precisely determined by the analysis of X-ray data. The amount of water in the interlayer space and the structure of the samples differed considerably in dependence on humidity. Convenient procedures and minimization strategy were established on the base of X-ray data in the molecular mechanic and the molecular dynamic simulations. A procedure for using of the supramol software was made. This software enables deterministic searching of conformational space. Initial models from supramol were minimized in the Cerius2 software using the Universal force field and then they were eventually optimized by the molecular dynamics. The arrangement of molecules of pyrenetetrasulphonate acid and water was determined in the interlayer space of hydrotalcite for three different samples with different interlayer distances: The sample 1 prepared by RH = 0%: 9.83A; the sample 2 prepared by RH = 84%: 13.63A; the sample 3 prepared RH = 40%–50%: 11.74A a 12.81A. The results of these structures proved a large variability of the arrangement of the molecules in the interlayer space. The sample No. 3 seems to be unstable.