THERMODYNAMIC COMPLEXING OF MONOCYCLOPENTADIENYLFERRUM (II) INTERCALATES WITH DOUBLE-WALLED CARBON NANOTUBES

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By employing the methods of molecular dynamics MM+, semi-empirical quantum-chemical PM3 and Monte-Carlo, there has been studied the positioning of monocyclopentadienylferrum (II) molecules in double-walled (5,5)@(10,10) carbon nanotubes (CNT) depending on their concentration and temperature. The molecules have been found out to form stable bonds with CNT walls, with a tendency between intercalate stability and the CNT structure. The temperature growth (over ~500 K) causes gradual bond ruining followed by extrusion of interwall intercalate. Further temperature increase up to 600-700 K is characterised with intercalate external surface desorption, stabilising the whole system and keeping the interwall intercalate only (Fig. 1). There have been calculated the CNT's UV-spectrum (5,5)@(10,10) depending on intercalate concentration and the association constant of the "double-walled CNT – intercalate" system which makes 6.745 $l \cdot mole^{-1}$. Thus, unique optical, electrical and magnetic behaviour of cyclopentadienyl complexes, their ability to form high-stable intercalate with CNT opens a prospect of their applying in non-linear optics and nanoelectronics.

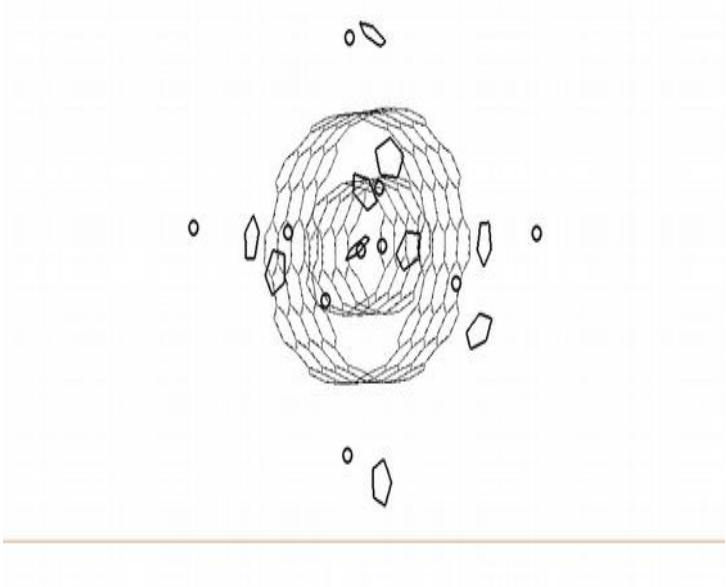

Fig. 1. Screenshot of configurational change of "double-walled CNT – intercalate" system being heated.