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研究论文

适用于液晶大分子的量子化学计算方法以及六烷氧基苯并菲取代的**1,3,5-**三酰胺苯液晶的研究

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摘要 盘状液晶分子之间的相互作用决定液晶的性质. 为了选择合适的计算方法,
以便用量子化学研究液晶大分子, 设计了对位取代苯和三酰胺苯作为模型分子, 用高水平的ONIOM [MP2/6-31G*(0.25):HF/6-31G(d,p)]计算提供了与晶体结构资料相符合的较准确的二体相互作用结果.
然后与各种较低级别的计算进行比较, 说明ONIOM (HF/STO-3G: AM1:UFF)水平比较合适.
盘重叠部分的相互作用主要是色散作用, 用UFF力场处理, 氢键主要是静电作用, 用HF/STO-3G处理,
其余部分用AM1处理. 通过对苯取代的1,3,5-三酰胺苯的双分子构型优化, 并与晶体结构数据进行比较,
进一步说明ONIOM (HF/STO-3G:AM1:UFF)水平计算的适用性. 在此基础上, 对六烷氧基苯并菲取代的1,3,5-三酰胺苯的双分子构型进行了优化, 为解释它所形成的液晶具有较高的电荷传输能力提供了有用的信息.

关键词 盘状液晶 电荷传输 量子化学 ONIOM方法

分类号

A Suitable Method for Quantum Chemical Calculations on Large Mesogen and the Study of 1,3,5-Benzenetrisamide Liquid Crystal Substituted with Three Hexaalkoxytriphenylene Groups

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Abstract The properties of discotic mesophases are determined by the interactions of molecules forming mesophases. It is difficult to do quantum chemical calculation on so large molecule pairs. Various level calculations have been performed on pairs of benzene derivatives and 1,3,5-benzenetrisamide. The results have been compared with those by high level ONIOM [MP2/6-31G*(0.25):HF/6-31G(d,p)] calculations, finding that the results with ONIOM (HF/STO-3G:AM1:UFF) level calculations are best. The hydrogen bond is dominated by the electrostatic contributions, well covered at the HF/STO-3G level. The stabilization of the stacked molecules was mostly assumed to be due to the dispersion energy, which could be estimated with a UFF method. Triphenyl substituted trimesamide is then optimized at ONIOM (HF/STO-3G:AM1:UFF) level, and the result is in good agreement with the crystallographic data. As an example, 1,3,5-benzenetrisamide with three pendant hexaalkoxytriphenylene groups has been calculated at ONIOM (HF/STO-3G: AM1:UFF) level. The results reported here supported the previous assumption about good charge transfer property of this liquid crystal.

Key words discotic liquid crystal charge transfer quantum chemistry ONIOM method

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