化学学报 1999 57 (4): 372-376 ISSN: 0567-7351 CN: 31-1320/06

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LB膜中NMOB分子构象的研究

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收稿日期 修回日期 网络版发布日期 接受日期

摘要 利用DFTB3LYP/4-31G^*方法,对2-硝基-5-(N-甲基-N-十八烷基)氨基苯甲酸(NMOB)进行研究。计算结果发现,苯环的5位碳原子、氨基氮原子以及十八烷基链上与其最临近的两个碳原子所组成的两面角(D)约为90iii时,NMOB有最稳构象,在NMOB自交替膜中,NMOB即以这种构象存在;而D=180iii时,体系总能量较最稳构象高出31.57kJ/mol,这种构象存在于NMOB/花生酸镉(CdA)交替膜中,较小的能量差异使NMOB容易在两种构象之间进行转化,在NMOB/花生酸镉(CdA)交替膜中因受到花生酸直立构象紧密排列的诱导作用,NMOB分子以能量相对较高的构象存在。

关键词 L-B膜 分子构象 苯甲酸P 苯胺P 从头计算法

分类号 0641

Theoretical study on the conformation of NMOB in LB films

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Abstract In this paper, the NMOB molecule is studied in terms of DFT B3LYP method using 4-31G^* basis set. The geometry of NMOB was obtained by replacing the ethyl in 2-nitro-5-(N-methyl-N-ethyl) amino benzoic acid (NMEB) whose geometry was optimized by B3LYP/3-21G^* with octadecyl from dimethyloctadecylamine (DMOA) optimized by PM3. We defined the dihedral angle as D, which was composed of the amino nitrogen atom, the carbon atom in benzene ring connecting directly to the amino nitrogen atom and the two carbon atoms in octadecyl group nearest to the nitrogen atom. It was found that the system potential curve had minimums when the D of NMOB was equal to about 90 iii or 270iii . There was a maximum at 180iii whose system potential was 31kJ/mol higher than that of 90iii and 28kJ/mol than that of 270iii (shown in Tab. 2 and Fig. 2). The most stable conformation of NMOB (D ≈90iii or 270iii) exists in its self-alternated multilayer. In NMOB/Cadmium arachidate (CdA) alternated film, NMOB exists in the form of vertical conformation (D=180iii). We suggested the unstable vertical conformation of NMOB come from the inducement of CdA, which stood, vertically on the substrate.

Key words L-B MEMBRANE MOLECULAR CONFORMATION BENZENECARBOXYLIC ACID P BENZAMINE P AB INITIO CALCULATION

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