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偶氮苯衍生物自组装单分子膜中的分子取响

张浩力,张锦,李海英,刘忠范,力虎林

兰州大学化学系.兰州(730000);抚顺石油学院石化系;北京大学化学与分子工 程学院智能材料研究中心

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摘要 利用反射红外光谱研究了金表面一系列具有不同碳链长度的偶氮苯巯基衍生物的自组装单分子膜.
通过对比各向同性样品的透射谱和单分子膜的反射谱中各个吸收峰强度,
定量地研究了分子中各部分的取向与分子结构的关系.我们分别提出了烷基链和偶氮基团取向计算的方法,
利用该方法成功地求得了分子中各部分在膜的倾角.结果显示,当分子中烷基链长度增大时,
碳链和偶氮苯基团相对于法线的倾斜逐渐加剧.这种倾角的变化归因于分子中碳链间范德华引力增大时,
引起分子逐渐倾斜以达到最佳的范德华接触.同时研究发现,烷基链和偶氮基团受碳长度变化的影响并不相同.
当分子中亚甲基数目增多时,烷基链的倾角迅速增大而偶氮苯倾角的增大则相对缓慢,
这反映了它们在空间需求和本身刚性上的不同。

关键词 苯偶氮化合物 分子取向 单分子膜 反射红外光谱

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Molecular orientation of self-assembled monolayers of azobenzene derivatives

Zhang Haoli,Zhang Jin,Li Haiying,Liu Zhongfan,Li Hulin

Lanzhou Univ, Dept Chem.Lanzhou(730000)

Abstract Self-assembled monolayers (SAM~s) of a series of azobenzene derivatives on gold were characterized with reflectance absorption infrared spectroscopy (RA-IR). The effect of molecular structure of azobenzene derivatives on molecular orientation of their SAM~s was investigated by comparison of the RA-IR spectra with the corresponding transmission spectra of the isotropic samples. Mathematical expressions were explored for orientation evaluation of the alkly chain and the azobenzene group, respectively. Our investigation reveals that both the alkyl chain and the azobenzene chromophore tilt away dramatically from the surface normal direction with lengthening of the alkly chain. The molecular orientation changes in the series of SAM~s were attributed to the changes of van der waals interaction among alkyl chains. The influences of alkyl chain lengthing on alkyl chain and azobenzene group are not the same. While the number of the methylene moiety in molecule increases, the tilting angle of alkyl chain increases rapid but the changes of tiltign angle of azobenzene moiety is relative insignificant. Such difference between alkyl chain and azobenzene group is attributed to difference in rigidity.

Key words BENZENE AZO COMPOUNDS MOLECULAR ORIENTATION MONOMOLECULAR FILMS

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通讯作者