研究论文

几个超分子体系中非常规键的AIM分析

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摘要 对五个含氟分子自组装形成的晶体进行了AIM (Atoms in Molecules)分析, 观察到、 并定量地描述了这些晶体中大量存在的氟原子相关的非常规弱相互作用力; 并且找到一个完全由F... O弱相互作用主导的超分子自组装晶体.

关键词 超分子 非常规键 氟原子 AIM分析

分类号

AIM Analysis of Unconventional Bonds in Some Supramolecular Systems

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Abstract Five crystals containing fluorine atoms were prepared. The electronic structures of these crystals were studied theoretically and a lot of unconventional weak interaction were found. Particularly, one of these crystals was self-assembled by overwhelming weak F...O bonds, not hydrogen bonds.

Key words supramolecule unconventional bond fluorine atom AIM analysis

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