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Full Papers

$C_{74}(BN)_2$的UV和IR 光谱研究

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摘要 用INDO系列方法研究了$C_{74}(BN)_2$的16种可能异构体的平衡构型，表明最稳定的三个异构体是硼和氮取代$C_{78}(C_{2v})$长轴附近同一六员环上的碳原子形成B-N-B-N单元。 用INDO/CIS方法计算了$C_{74}(BN)_2$的电子光谱，讨论了$C_{74}(BN)_2$的UV吸收峰与$C_{78}(C_{2v})$相比发生红移的原因。在AM1优化构型基础上，计算了9,8,28,29-$C_{74}(BN)_2$和28,29,30,31-$C_{74}(BN)_2$的红外光谱。

关键词 $C_{74}(BN)_2$, 电子光谱, 红外光谱, 红移

分类号

Investigation on UV and IR Spectra of $C_{74}(BN)_2$

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Abstract Equilibrium geometries of 16 possible isomers for $C_{74}(BN)_2$ were studied by INDO series of methods, to indicate that the most stable three geometries are those where boron and nitrogen atoms substitute carbon atoms located at the same hexagon near the longest axis of C_{78} (C_{2v}) to form B-N-B-N unit. Electronic spectra of $C_{74}(BN)_2$ were investigated with INDO/CIS method. The reason for the red shift of UV absorptions for $C_{74}(BN)_2$ compared with those of C_{78} (C_{2v}) was discussed. IR spectra for 9,8,28,29-$C_{74}(BN)_2$ and 28,29,30,31-$C_{74}(BN)_2$ were calculated on the basis of AM1 geometries.

Key words $C_{74}(BN)_2$, electronic spectra IR spectra red shift

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