

## 几种 $C_{70}^n$ 离子的 Jahn-Teller 畸变和单态的电子光谱

滕启文, 吴师, 赵学庄, 唐敖庆, 封继康

南开大学化学系; 吉林大学理论化学研究所

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**摘要** 用 INDO 系列方法对  $C_{70}^n$  ( $n=+2, +1, -1, -2, -3, -4$ ) 进行系统研究, 表明除  $C_{70}^n$  三态具有  $D_{5h}$  对称性, 其余均发生 Jahn-Teller 畸变, 导致明显的对称性降低 ( $C_{2v}$ ), 产生 30 种键长和 21 种不同 C 原子。以优化构型为基础, 计算  $C_{70}^{4-}$  单态的电子光谱, 其近红外吸收与实验值一致, 同时预测了  $C_{70}^{2+}$  单态的光谱。

**关键词** [微分重叠间忽略近似](#) [电子光谱](#) [碳七十](#)

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## The Jahn-Teller distortion of several $C_{70}^n$ ions and electronic spectra for singlets

TENG QIWEN, WU SHI, ZHAO XUEZHUANG, TANG AOQING, FENG JIKANG

**Abstract** The INDO methods were used to perform theoretical studies for  $C_{70}^n$  ( $n=+2, +1, -1, -2, -3$  and  $-4$ ). It was shown that the Jahn-Teller distortion has taken place for  $C_{70}^n$  except for  $C_{70}^{2+}$  triplet ( $D_{5h}$ ), which results in the lowering of symmetry to  $C_{2v}$  and produces 30 kinds of bonds and 21 unique carbon atoms. Based on the optimised geometries, the electronic spectrum for  $C_{70}^{4-}$  singlet was calculated, the NIR absorptions of which are good agreement with the experimental results. Meanwhile the electronic spectrum for  $C_{70}^{2+}$  singlet was predicted.

**Key words** [INTERMEDIATE NEGLECT OF DIFFERENTIAL OVERLAP APPROXIMATION \(IND ELECTRONIC SPECTROSCOPY\)](#)

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