

咪唑及其N-取代衍生物的气相He I紫外光电子能谱与量子化学研究

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**摘要** 首次系列报道了9-H咪唑及其系列N-取代衍生物的气相HeI紫外光电子能谱,借助于Gauss-94采用RHF/3-21G基组对它们的几何构型进行优化,并用RHF/6-31G基组计算分子轨道及能级,

计算的分子轨道特征和能量很好地反映了各谱带的特点和分子间电离能的变化规律。依计算结果,

以及同系列分子间谱带及相应电离能的相互比较,对每个分子的UPS谱带给予指认,讨论了N-烷基化对 $\pi$ 分子轨道的选择性去稳定化作用,并讨论了分子之间电离能的变化规律,得到一系列有益的结论。

**关键词** [咪唑](#) [氦](#) [紫外光电子谱法](#) [几何异构](#) [分子轨道](#)

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## Studies of 9-H carbazole and its N-substituted derivatives by He I ultraviolet photoelectron spectroscopy and quantum chemistry

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**Abstract** Gas-phase HeI ultraviolet photoelectron spectra (UPS) of 9-H carbazole and N-substituted derivatives are reported in this paper. The property and the eigenvalue of each related molecular orbital obtained from the calculations are well consistent with the character of spectra bands and the changing rules of I~v between carbazole and N-substituted carbazole. In addition to the assignment of the spectra, some useful conclusions were obtained: comparing the N-alkylated derivatives with the parent carbazole, the  $\pi$  orbitals' character on the carbazole ring have no change; only the related ionization potentials (IPs) shift to lower energy, this is, the selective destabilization of the  $\pi$  orbitals. Increasing the carbon atom number in the n-alkyl has little effect on the  $\pi$  orbitals' character and their IPs, nor does the substitution site of the alkyls. The selective destabilization has main effect on the  $\pi$  orbitals which largely located on the nitrogen atom.

**Key words** [IMIDAZOLE](#) [HELIUM](#) [GEOMETRICAL ISOMERISM](#) [MOLECULAR ORBIT](#)

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