

系列二羰基化合物的HeI紫外光电子能谱(UPS)及量子化学研究

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摘要 报道了醌及苯并酸酐等系列二羰基化合物的气相HeI紫外光电子能谱。对各体系利用Gaussian94程序RHF/3-21G进行了构型优化,对得到的优势构型采用STO-

6G基组进行了轨道计算。并结合计算结果对各分子体系的UPS谱进行了分析指认。计算结果分析显示:标题化合物的第一个电离峰均是由苯环部分的共轭 π 键电子电离及羰基的孤对电子电离引起的,且化合物的IP~1值随羰基在HOMO轨道中权重的增大而增大。各化合物的第二、三谱带都与羰基不同类型的孤对电子峰相关联。说明羰基为此类化合物的特征基团。且分子的对称性越高,羰基的孤对电子峰 n^- 和 n^+ 的平均值越大,分裂值也越大。

关键词 [羰基化合物](#) [紫外光电子谱法](#) [醌](#) [酸酐](#)

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HeI photoelectron spectroscopy and theoretical studies of the series of dicarbonyl compounds

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Abstract The HeI photoelectron spectroscopy of compounds 1, 4-Naphthoquinone, tetracyano-benzoguinone, di-*o*-phthalic anhydride acid have been studied for the first time. To assign these spectra, RHF/3-21G optimization and RHF/STO-6G molecular orbital calculation for these three compounds have also been performed. The results show that: the first ionization peak of these compounds are all related to the π bonds of the benzene ring and carbonyl, and the increase of the ionization potentials of HOMO is linear with the gradual addition of the carbonyl in the HOMO. The second peak and the third peak of the three compounds are all related to the lone pair ionization of atom O. From these, we can conclude that: the carbonyl is the characteristics group of this kind of compound. Furthermore we also find that: the higher symmetry the compound has, the greater the average of n^-/n^+ is, and the greater n^- , n^+ splitting it has too.

Key words [CARBONYL COMPOUNDS](#) [QUINONE](#) [ACID ANHYDRIDE](#)

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