

研究论文

N-亚硝基吡啶系列化合物及其自由基负离子在乙腈介质中N—NO键断裂能的测定

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摘要 利用滴定量热技术并结合适当的热力学循环测定了乙腈溶液中7个取代的*N*-亚硝基吡啶化合物中N—NO键的异裂能和均裂能, 能量范围分别为206.1~246.2 kJ/mol和119.1~124.6 kJ/mol. 表明*N*-亚硝基吡啶均裂释放NO自由基(NO[•])比异裂释放NO正离子(NO⁺)要容易得多, 通过热力学循环得到的相应自由基负离子中N—NO键的异裂能和均裂能的能量范围分别为25.5~34.4和5.0~40.5 kJ/mol, 表明所研究化合物的自由基负离子在室温下很不稳定.

关键词 [N-亚硝基吡啶](#) [N-亚硝基吡啶自由基负离子](#) [N—NO键能](#) [滴定量热](#)

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Determination of N—NO Bond Dissociation Energies of *N*-Nitrosoindoles and Their Radical Anions in Acetonitrile

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Abstract The heterolytic and homolytic N—NO bond dissociation energies of seven *N*-nitrosoindole derivatives were evaluated by using titration calorimetry and relative thermodynamic cycles. The energetic scales of the heterolytic and homolytic N—NO bond dissociation energies of *N*-nitrosoindoles cover the ranges from 206.1 to 246.2 kJ/mol and from 119.1 to 124.6 kJ/mol, respectively, which indicates that *N*-nitrosoindoles are much easier to release a NO radical(NO[•]) rather than a NO cation(NO⁺). The estimation of the heterolytic and homolytic(N—NO)^{•-} bond dissociation energies of the *N*-nitrosoindoles radical anions gives the energetic ranges from 25.5 to 33.4 kJ/mol and from 5.0 to 40.5 kJ/mol for the(N—NO)^{•-} bond homolysis and heterolysis, respectively, which means that *N*-nitrosoindole radical anions are unstable at room temperature.

Key words [N-Nitrosoindoles](#); [Radical anions of N-nitrosoindoles](#); [N—NO bond energy](#); [Titration calorimetry](#)

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