Chinese Journal of Chemistry 2005 23 (8): 1053-1059 ISSN: 0567-7351 CN: 31-1320/06

FULL PAPERS

MALDI/FTMS中碰撞衰减机理对准确质量校正的影响

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收稿日期 2004-10-10 修回日期 2005-4-29 网络版发布日期 接受日期

摘要 本文从系统模式特征方程Force (是摩擦衰减力)推导出了质量校正方程 $m/z=A/\{f+m_{neutral}k/[m^{\wedge}+m_{neutral}]\}+B/f\{f+m_{neutral}k/[m^{\wedge}+m_{neutral}]\}$，
其中k是外标法校正中根据基质离子或其它已知离子观测频率的变化而改变的修正比例系数。通过阿奇霉素降解产物实验验证并揭示了新的校正方程的有效性及准确性。质量测定相对误差均小于2×10^{-6}。

关键词 基质辅助激光解吸离子化, 傅立叶变换质谱, 碰撞衰减机理, 质量校正

分类号

Effect of Damping Mechanisms on Mass Calibration Equation for MALDI/FTMS

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Abstract Collisional damping affects the relationship between ion mass and effective cyclotron frequency in Fourier transform mass spectrometry. The exact mass calibration equation $m/z=A/\{f+m_{neutral}k/[m^{\wedge}+m_{neutral}]\}+B/f\{f+m_{neutral}k/[m^{\wedge}+m_{neutral}]\}$ was therefore derived from the characteristic equation of system model, force=m(dv/dt)=$qE-qv\times B_0-\xi v$), (ξv, a frictional damping force), in which k is amended by the shift of observed frequency of matrix ion or other known ion in external calibration. The mass obtained by the amended calibration equation is therefore immune to collisional damping and space-charge effects on mass accuracy. The relative errors of ion mass measured were all less than 2×10^{-6}.

Key words MALDI FTMS damping mechanism mass calibration

DOI:

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