

## Detection of Optical Stability of chiral 2-Methylbutyric Acid in Gas Phase with Quadrupole-Quistor-Quadrupole Mass Spectrometer

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**Abstract:** Optical stability of chiral 2-methylbutyric acid in gas phase has been detected with Quadrupole-Quistor-Quadrupole tandem mass spectrometer in combination with deuteration. The results show that these compounds are optically unstable in the process of self chemical ionization.

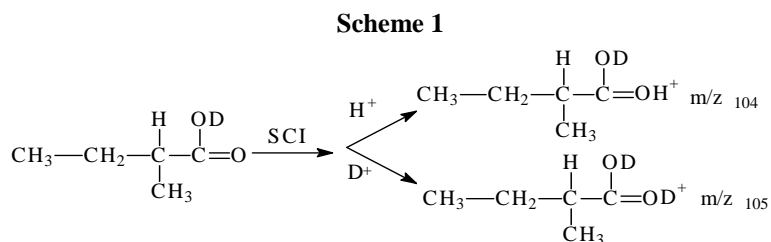
**Keywords:** 2-Methylbutyric acid, optical stability, mass spectrometric detection.

In our previous work<sup>1</sup>, we have investigated the optical stability of organic acid enantiomers which possess one  $\alpha$ -hydrogen at the chiral carbon of the molecule during Electron Impact ionization Mass Spectrometry (EI-MS) process, the study showed these compounds are optically stable in the process of instantaneous vaporization at high temperature and electron impact ionization. Here we report the results from Self Chemical Ionization Mass Spectrometry (Self CIMS) process.

The measurements were performed with purposed-built quadrupole-quistor-quadrupole tandem mass spectrometer. EI energy was 70eV, the temperature of the ion source was about 200°C. Mass spectrometric data were recorded on AT personal computer.

**Chemicals:** 2-methylbutyric acid and deuterated methanol were used as purchased, carbonyl group deuterated 2-methylbutyric acid was obtained from deuterium exchange.

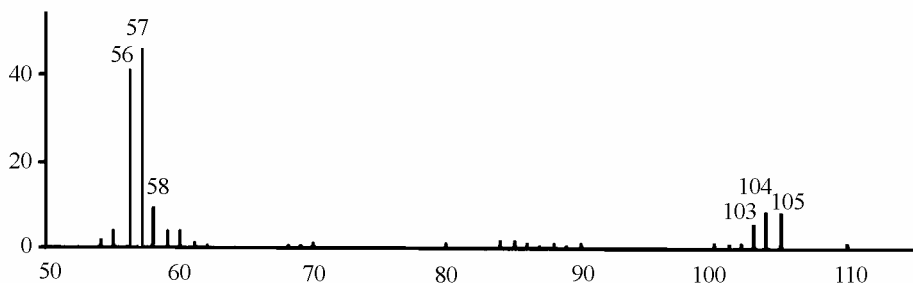
Under self chemical ionization, deuterated 2-methylbutyric acid yields two types of pseudo-molecular ions ( $m/z$  104 and  $m/z$  105) from the reaction as below:



If enolization does not occur during the self-CI MS process (in gas phase) of deuterated 2-methylbutyric acid, the major characteristic fragment ion (the capture of the carbonyl group) would lead to the presence of ion peak at  $m/z$  57

$[\text{CH}_3\text{CH}_2\text{C}^+(\text{H})(\text{CH}_3)]$  in the mass spectrum, and the relative abundance of the corresponding ion peak at  $m/z$  58 resulting from the contribution of  $^{13}\text{C}$  isotope is about 5% (the ratio of 58/57), which is just like the situation of in EIMS<sup>1</sup>. But from the self CI mass spectrum of deuterated 2-methylbutyric acid (**Figure 1**), it can be seen that the ratio of 58/57 is about 20%, this high ratio could result from the enolization occurring in the self-CI MS process of deuterated 2-methylbutyric acid, in which the  $\alpha$ -H was exchanged with deuterium from carbonyl group. This deduction was proved by CID experiments. The CID spectrum of the selected ions at  $m/z$  104 shows that the ratio of 58/57 is 23%, and the CID spectrum of the selected ions at  $m/z$  105 shows that the ratio 58/57 is about 60. These high ratios of 58/57 no doubt indicate that the ions at  $m/z$  58 mainly result from the fragment of  $\text{CH}_3\text{CH}_2\text{C}^+(\text{D})(\text{CH}_3)$  and this also suggests enolization indeed occurred in the gas phase during the self chemical ionization process because of the existence of the proton acid which acts as the catalyst of enolization reaction in gas phase, this also suggests these compounds are optically unstable in self-CI MS process.

**Figure 1.** Mass spectrum of deuterated 2-methylbutyric acid



## Reference

1. Y. J. Pan, U. P. Schlunegger ; *Proceedings of 45<sup>th</sup> ASMS conference*, June, 1997, California, Palm Springs, USA

Received 21 August 1998