Rapid Detection of Multiple Gas Mixtures and Evaluation of Harmful Gas Removal Efficiency in Deck Decompression Chamber Using Dynamic Switching Mass Spectrometry

Qu Liang[a, 1], Pingxiao Liu[d, 1], Lei Zhao[c, *], Xuejun Wang[c], Jun Zou[c], Xun Bao[a], Qiangling Zhang[a], Wei Xu[a], Xue Zou[a], Shifeng Wang[d, *], Chaoqun Huang[a], Chengyin Shen[a, b, *], Yannan Chu[a, b]

[a]Anhui Province Key Laboratory of Medical Physics and Technology, Institute of Health and Medical Technology, Hefei Institutes of Physical Science, Chinese Academy of Sciences, Hefei, 230031, P.R. China

[b]Hefei Cancer Hospital, Chinese Academy of Sciences, Hefei, 230031, P.R. China

[c]No.719 Research Institute, China State Shipbuilding Corporation, 430200, Wuhan, P.R. China

[d] Naval Medical Research Institute, Shanghai, 200433, P.R. China

*Corresponding author; [1] Qu Liang, Pingxiao Liu, and Lei Zhao contributed equally to this work.

We performed targeted experiments using photoionization chemical ionization mass spectrometry (pCI-MS) and measured the full spectra of N_2 (as background), H_2S, and NH_3. The experimental results are as follows:

H_2S measurement experiment: As shown in Fig.S1 (a), when detecting H_2S, the signal intensity of H_3O^+ reached 3.08×10^6 cps, which clearly stands out as a dominant peak in the mass spectrum. Compared to the N_2 background spectrum, the signal intensity of the $H_2S{\bullet}H^+$ peak increased by 83-fold after introducing H_2S, confirming that H_2S undergoes ionization primarily through proton transfer with H_3O^+.

NH_3 measurement experiment: As shown in Fig.S1 (b), when detecting NH_3, the signal intensity of H_3O^+ was 1.93×10^6 cps, again appearing as a strong characteristic peak in the mass spectrum. Compared to the N_2 background spectrum, the signal intensity of the $NH_3{\bullet}H^+$ peak increased by 4.74-fold after introducing NH_3, indicating that NH_3 also ionizes via proton transfer with H_3O^+.

These experimental results clearly demonstrate that, under our measurement conditions, H_3O^+ indeed acts as the primary ionization reagent, exhibiting the highest signal intensity among all detected ions. Furthermore, the protonated products of H_2S and NH_3 ($H_2S{\bullet}H^+$ and $NH_3{\bullet}H^+$) are indeed generated through proton transfer reactions with H_3O^+.

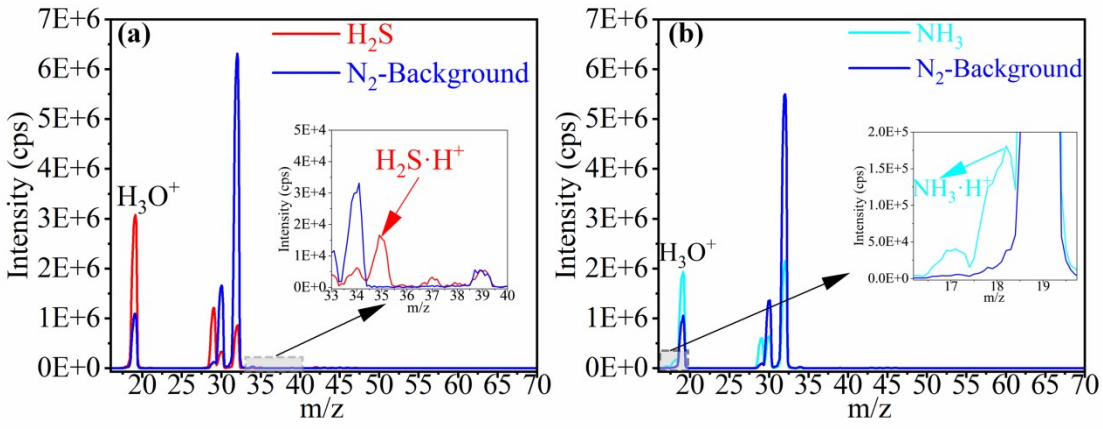

Fig. S1. (a) pCI-MS spectrum of H_2S; (b) pCI-MS spectrum of NH_3.

To demonstrate the characteristics of the dual-ion-source system, we compared the performance of pCI-MS and EI-MS in detecting representative target compounds in Fig. S2. As shown in Fig. S2 (a), when analyzing H_2S (with N_2 as the carrier gas),

the pCI-MS demonstrated superior performance, generating a prominent signal at m/z 35 ($H_2S•H^+$). Under identical conditions, the EI-MS failed to effectively detect the characteristic peak of H_2S (m/z 34). However, in a complementary manner, the EI-MS exhibited significant response to N_2, while the pCI-MS showed negligible variation.

Similarly, in Fig. S2 (b), during NH_3 detection (with N_2 as the carrier gas), the pCI-MS produced an intense signal at m/z 18 ($NH_3•H^+$), along with an NH_3^+ signal at m/z 17. Although the EI-MS displayed responses at the same m/z values, verification (Fig. S2 (b)-II) confirmed that these signals predominantly originated from background interference rather than NH_3.

The pCI-MS exhibited higher selectivity and sensitivity for polar molecules (e.g., H_2S and NH_3) while effectively suppressing background gas interference. Conversely, the EI mode proved more suitable for detecting inorganic gases such as N_2.

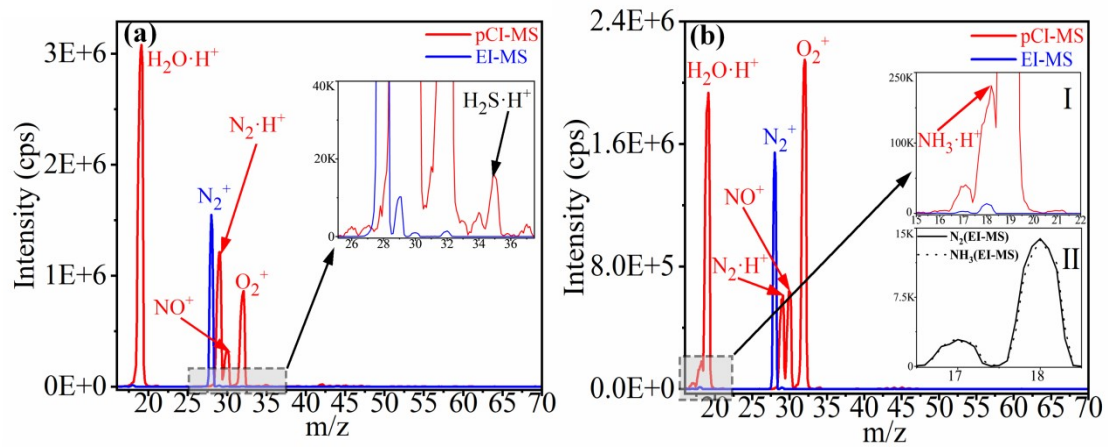

Fig. S2. (a) Fig. 2 (a) Comparison of pCI-MS and EI-MS spectrum for H_2S; (b) Comparison of pCI-MS and EI-MS spectrum for NH_3.