

Supplementary Material for

Solution- and gas-phase behavior of decavanadate: implications for mass spectrometric analysis of redox-active polyoxometalates

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Figure S4. Mass spectra of fragment ions produced by collisional activation of $\text{H}_4\text{V}_{10}\text{O}_{28}^{2-}$ (a 10-m/z unit mass selection window centered on the most abundant isotopolog).

Table S1. Table of m/z values, abundance values, and molecular formulas of assigned peaks labeled in Figure 1.

Table S2. Table of m/z values, abundance values, and molecular formulas of assigned peaks labeled in Figure 3.

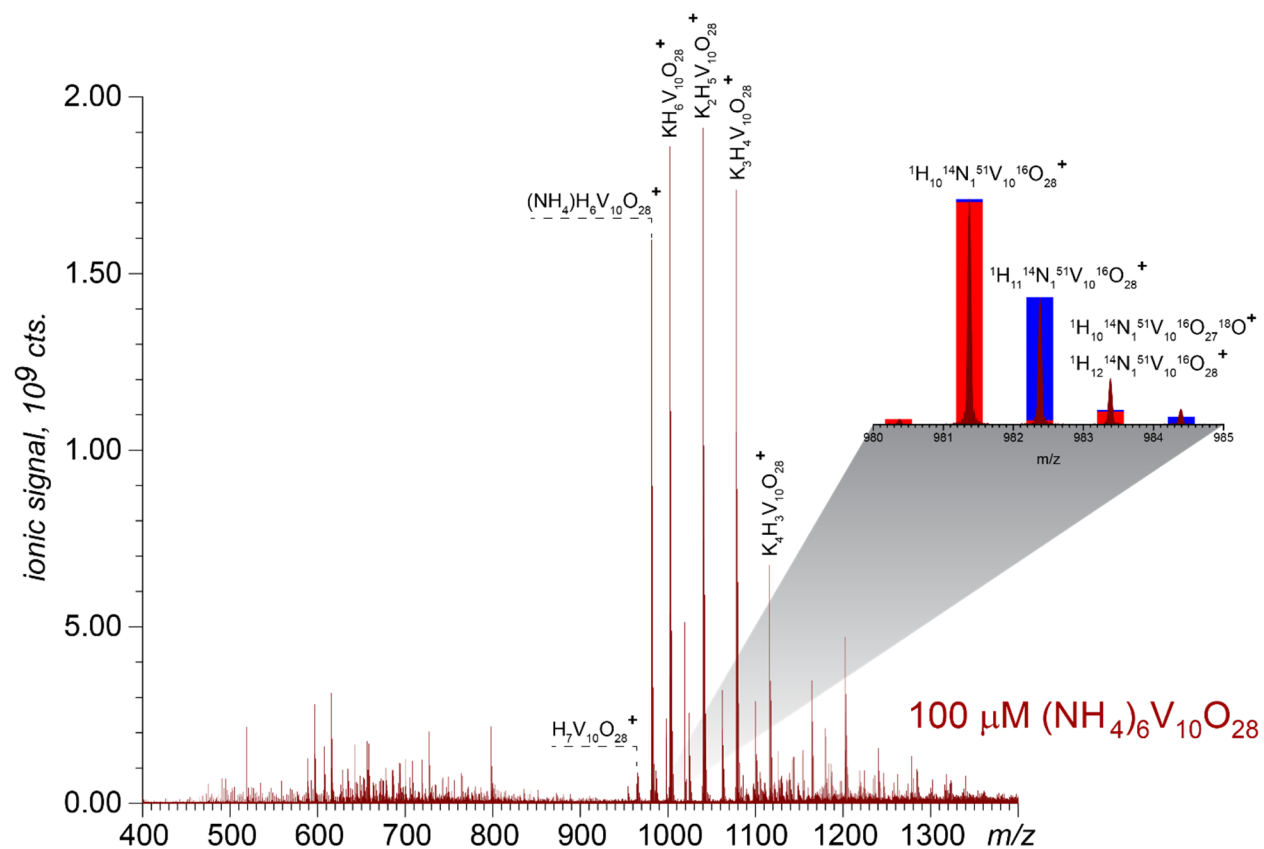
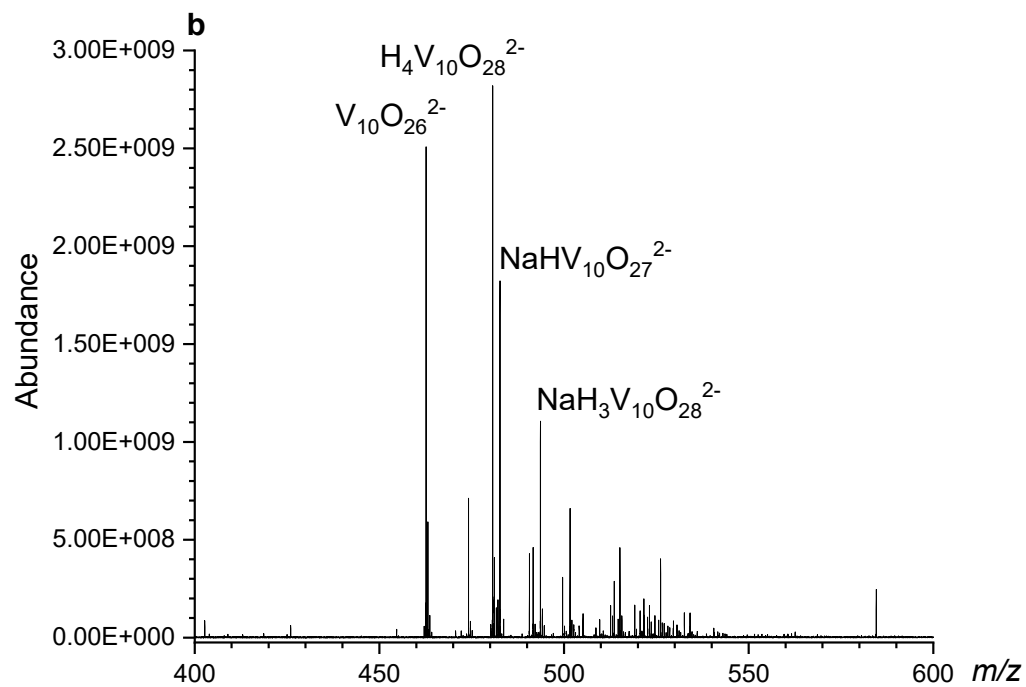
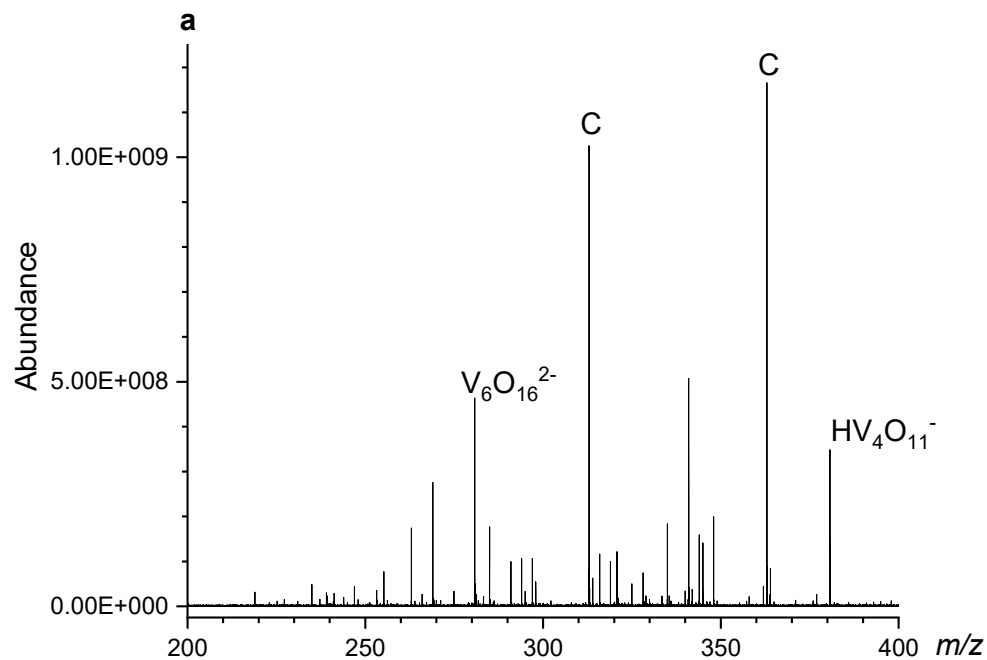
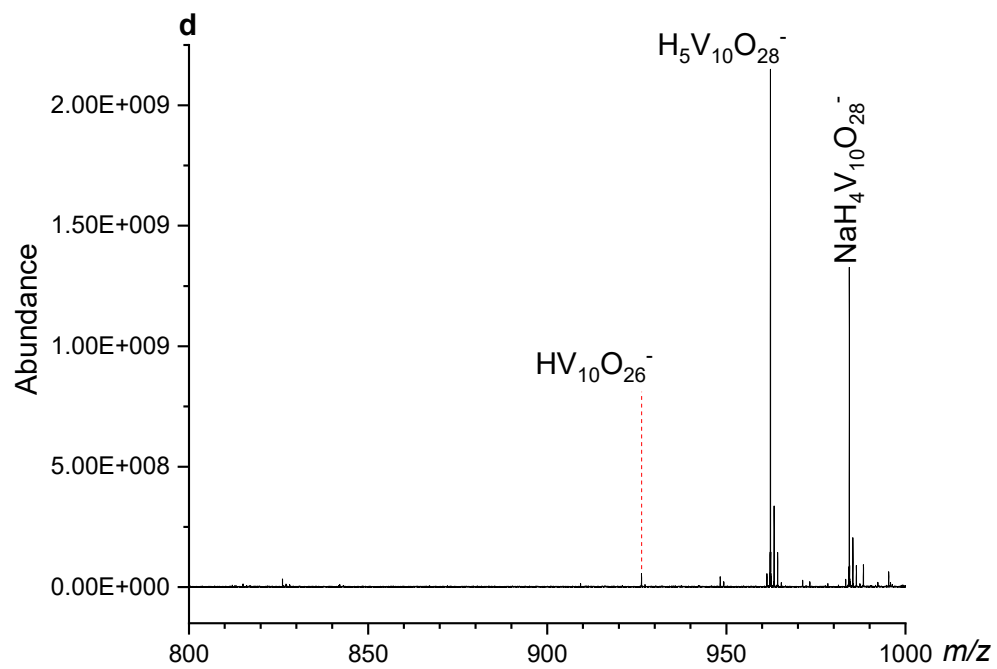
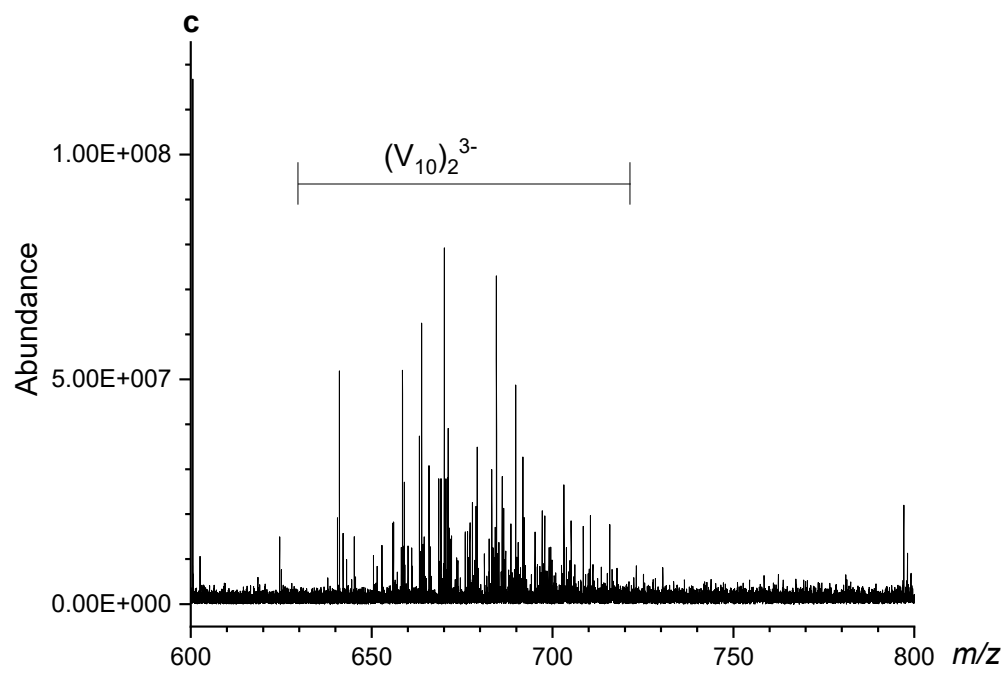


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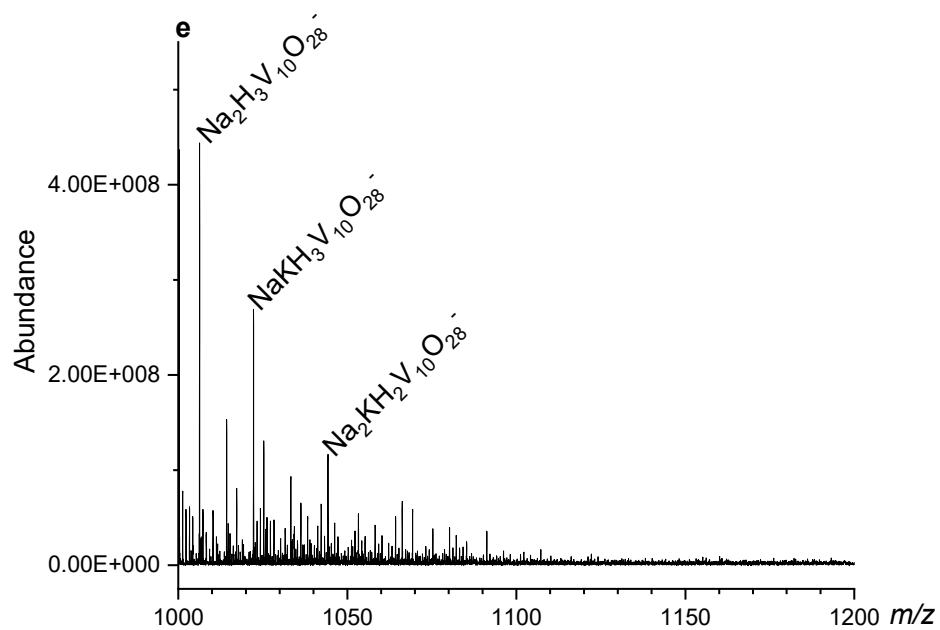


Figure S2. (a-e) Zoomed view of **Figure 1** containing 200-400 m/z (a), 400-600 m/z (b), 600-800 m/z (c), 800-1000 m/z (d), and 1000-1200 m/z (e).

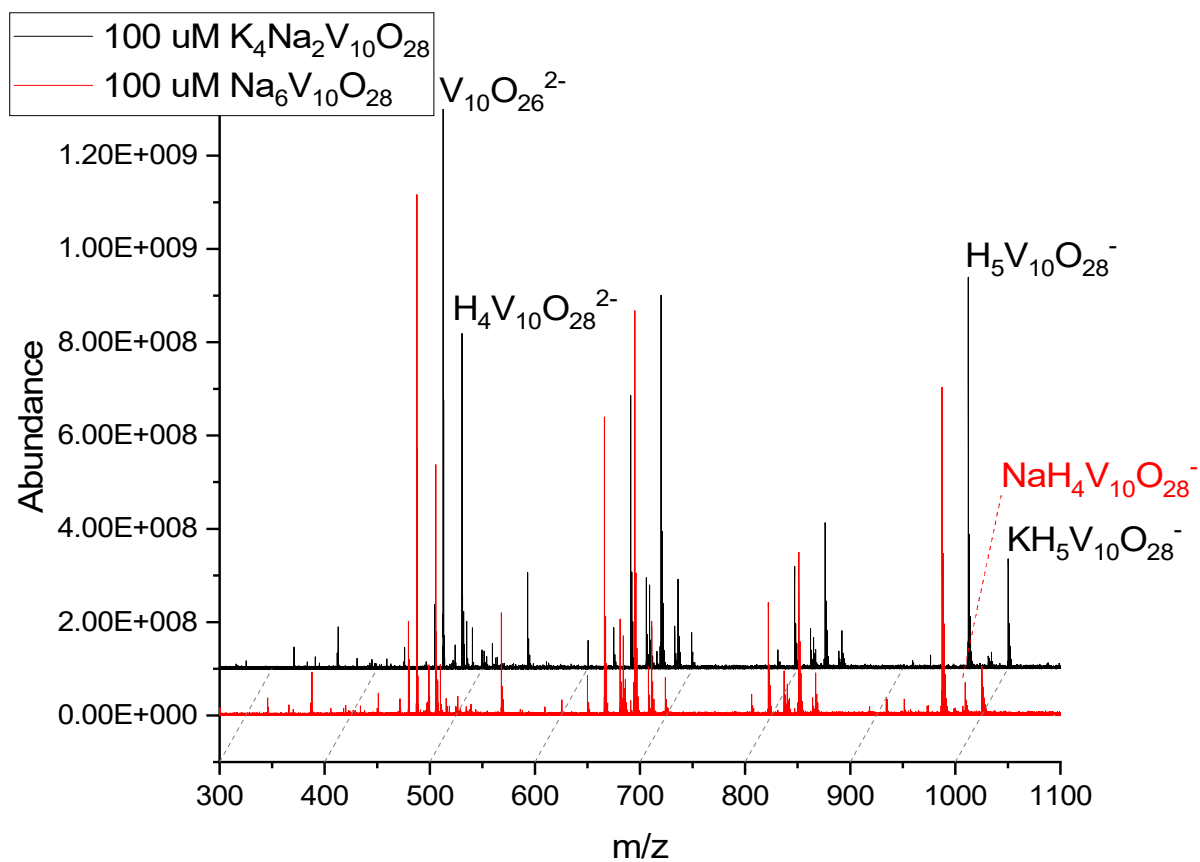
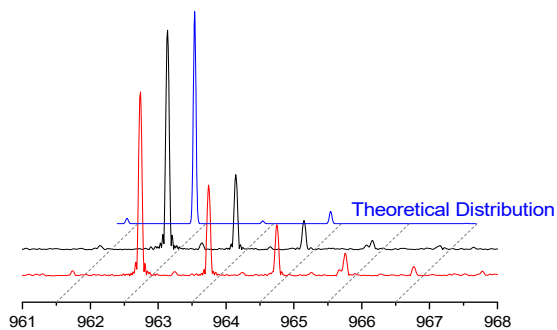


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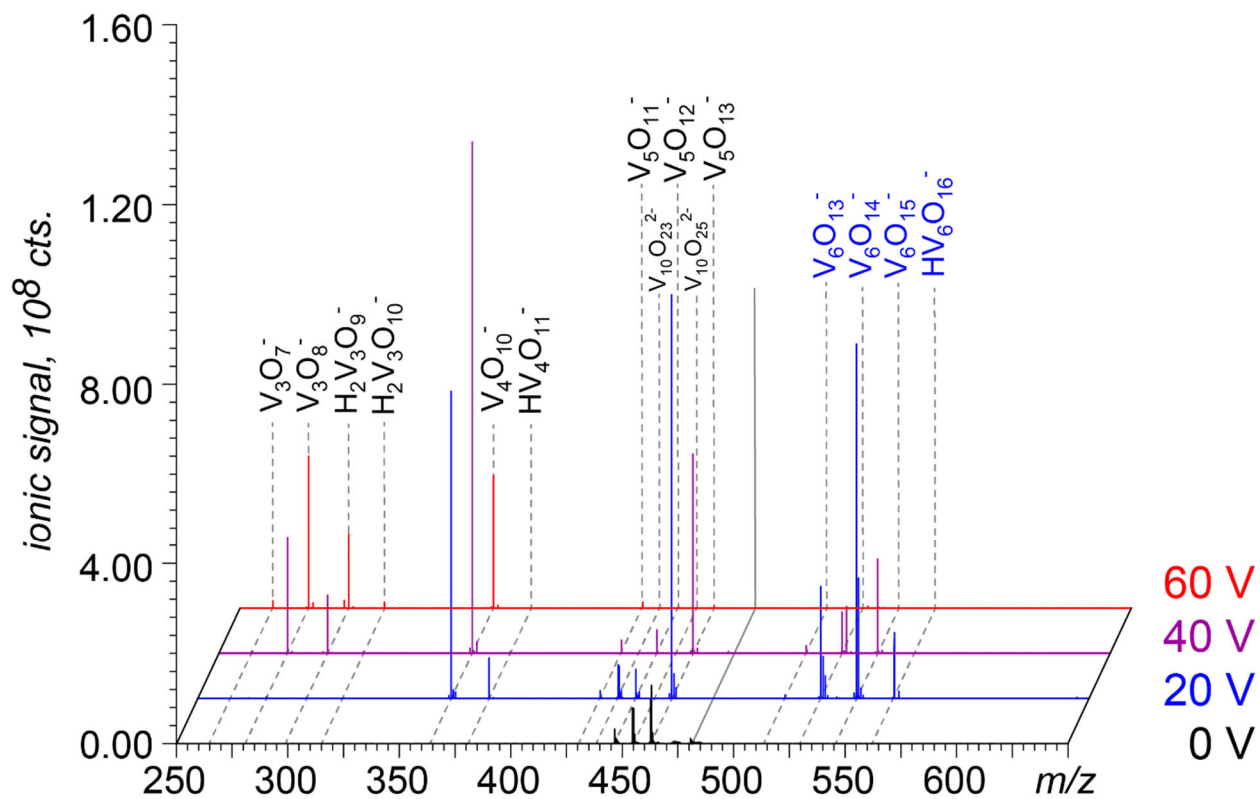


Figure S4. Mass spectra of fragment ions produced by collisional activation of $\text{H}_4\text{V}_{10}\text{O}_{28}^{2-}$ (a 10- m/z unit mass selection window centered on the most abundant isotopolog).

Table S1. Table of m/z values, abundance values, and molecular formulas of assigned peaks labeled in Figure 1.

m/z	Abundance	Assignment
280.79181	463657760	$V_6O_{16}^{2-}$
380.72834	348287360	$HV_4O_{11}^-$
402.71042	86153448	$NaV_4O_{11}^-$
454.65697	41454484	$V_{10}O_{25}^{2-}$
462.65415	2507207936	$V_{10}O_{26}^{2-}$
480.66477	2819456768	$H_4V_{10}O_{28}^{2-}$
491.65596	460635648	$NaH_3V_{10}O_{28}^{2-}$
909.31335	15266076	$V_{10}O_{25}^-$
926.31722	55977468	$HV_{10}O_{26}^-$
948.29856	43151184	$NaV_{10}O_{26}^-$
961.3389	54973988	$H_5^{50}V_1^{51}V_9^{16}O_{28}^-$
962.33733	2149368832	$H_5^{51}V_{10}^{16}O_{28}^-$
963.34409	336441952	$H_6^{51}V^{(V)}_9^{51}V^{(IV)}_1^{16}O_{28}^-$
964.3425	143054736	$H_5^{51}V_{10}^{16}O_{27}^{18}O_1^- / H_7^{51}V^{(V)}_8^{51}V^{(IV)}_2^{16}O_{28}^-$
965.3452	18526682	$H_6^{51}V^{(V)}_9^{51}V^{(IV)}_1^{16}O_{27}^{18}O_1^-$
984.32005	1326984192	$NaH_4V_{10}O_{28}^-$
1000.29332	436956064	$KH_4V_{10}O_{28}^-$
1006.29836	443729952	$Na_2H_3V_{10}O_{28}^-$
1022.27253	269013696	$NaKH_3V_{10}O_{28}^-$

Table S2. Table of m/z values, abundance values, and molecular formulas of assigned peaks labeled in Figure 3.

MSMS NaH ₄ V ₁₀ O ₂₈ ⁻		
m/z	Abundance	Assignment
932.29868	24559972	NaV ₁₀ O ₂₅ ⁻
948.29585	2927228672	NaV ₁₀ O ₂₆ ⁻
984.31444	7289208	NaH ₄ V ₁₀ O ₂₈ ⁻
MSMS H ₅ V ₁₀ O ₂₈ ⁻		
m/z	I	Assignment
909.31073	634640256	V ₁₀ O ₂₅ ⁻
926.31386	5410646528	HV ₁₀ O ₂₆ ⁻
962.33469	138024608	H ₅ V ₁₀ O ₂₈ ⁻
MSMS H ₄ V ₁₀ O ₂₈ ²⁻		
m/z	I	Assignment
454.65651	119309936	V ₁₀ O ₂₅ ²⁻
462.65375	10193562624	V ₁₀ O ₂₆ ²⁻
480.66433	126364768	H ₄ V ₁₀ O ₂₈ ²⁻