

**Lead(II)-Catalyzed Oxidation of Guanine in Solution
Studied with Electrospray Ionization Mass Spectrometry**

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Supporting Information

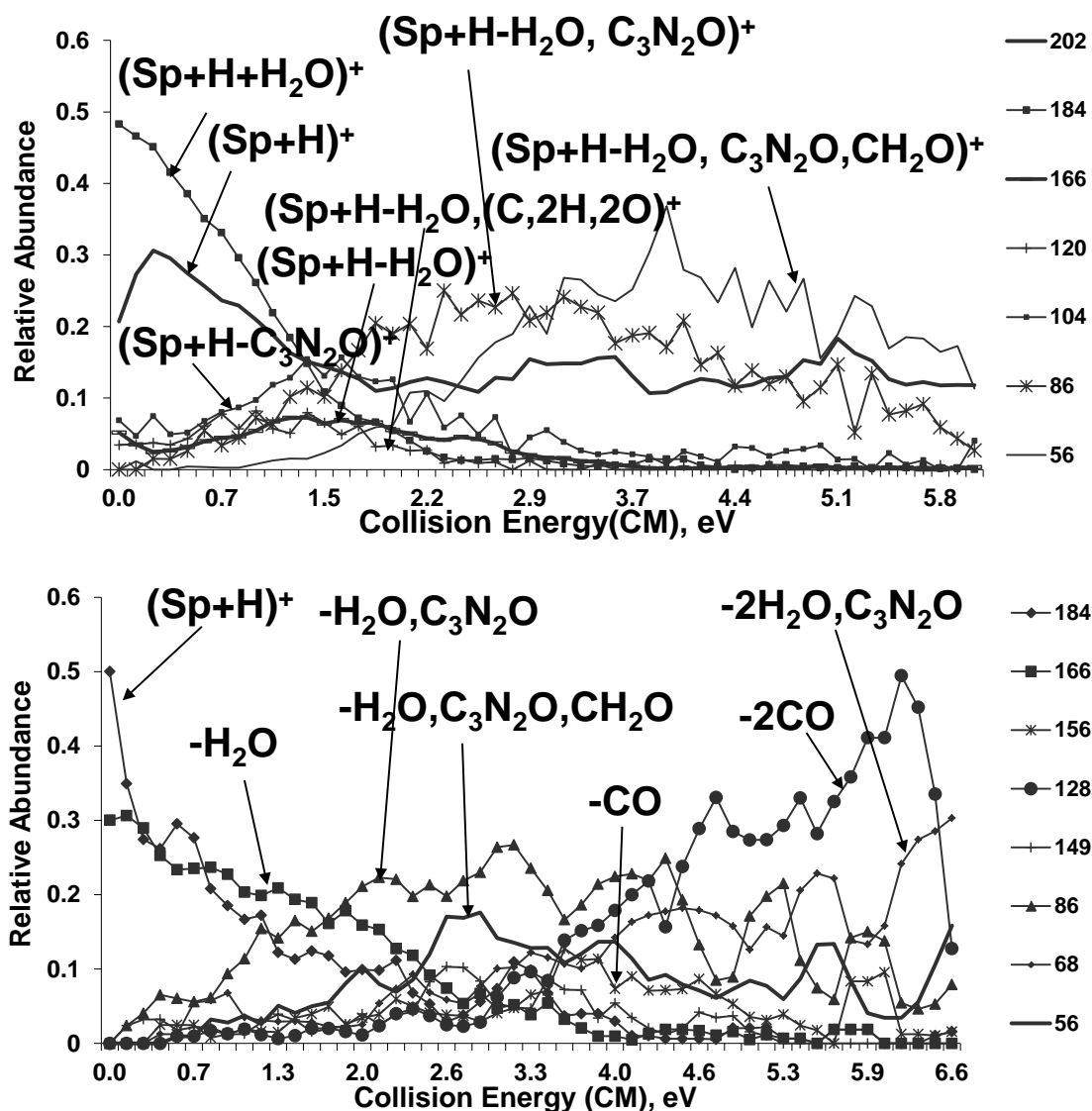


Figure S1. Dissociation profile for the product ions observed in oxidation of guanine by peroxymonosulfuric acid: $(\text{Sp}+\text{H}+\text{H}_2\text{O})^+$ (top) and $(\text{Sp}+\text{H})^+$ (bottom). The early onset of water loss in $(\text{Sp}+\text{H}+\text{H}_2\text{O})^+$ and commonality in the dissociation channels observed (predominant loss of H_2O and $\text{C}_3\text{N}_2\text{O}$ from the $(\text{Sp}+\text{H})^+$ ion) indicate that the water adduct is likely the proton-bound cluster formed in the electrospray and not a product of an in-solution reaction.

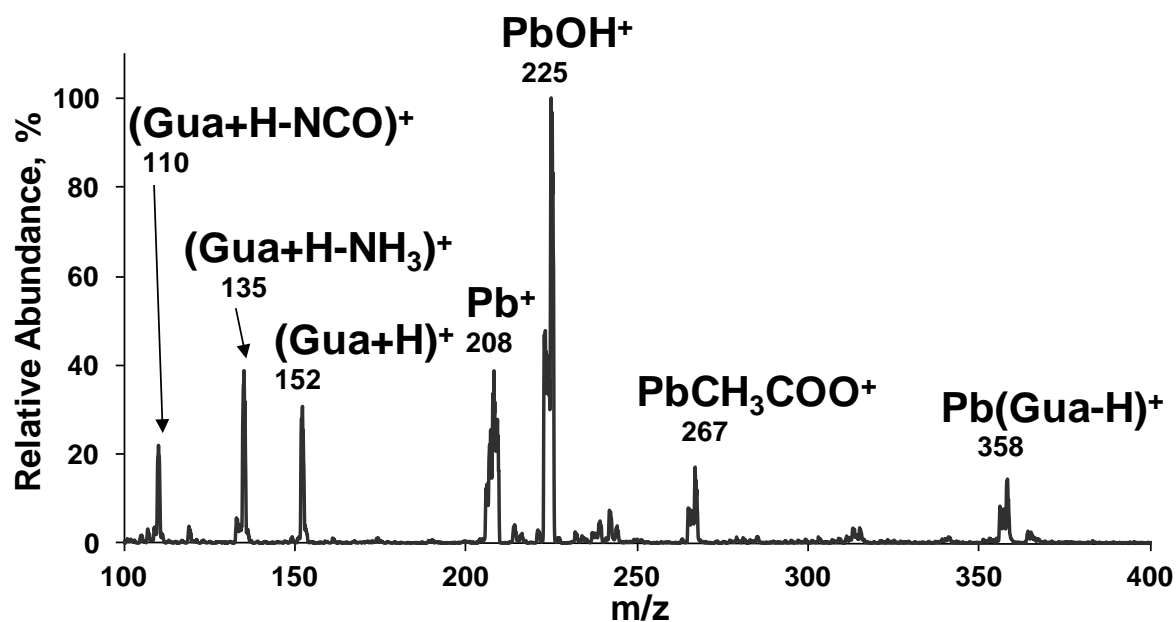


Figure S2. Mass spectrum for a solution containing guanine (Gua, 100 μ M) and lead acetate (1 mM). The observed products are: the lead(II)/deprotonated guanine complex [Pb(Gua-H)]⁺, protonated guanine (Gua+H)⁺ and its in-source fragmentation products (Gua+H-NH₃)⁺ and (Gua+H-NCO)⁺ as well as lead monoacetate, lead mono-hydroxide and the lead cation.

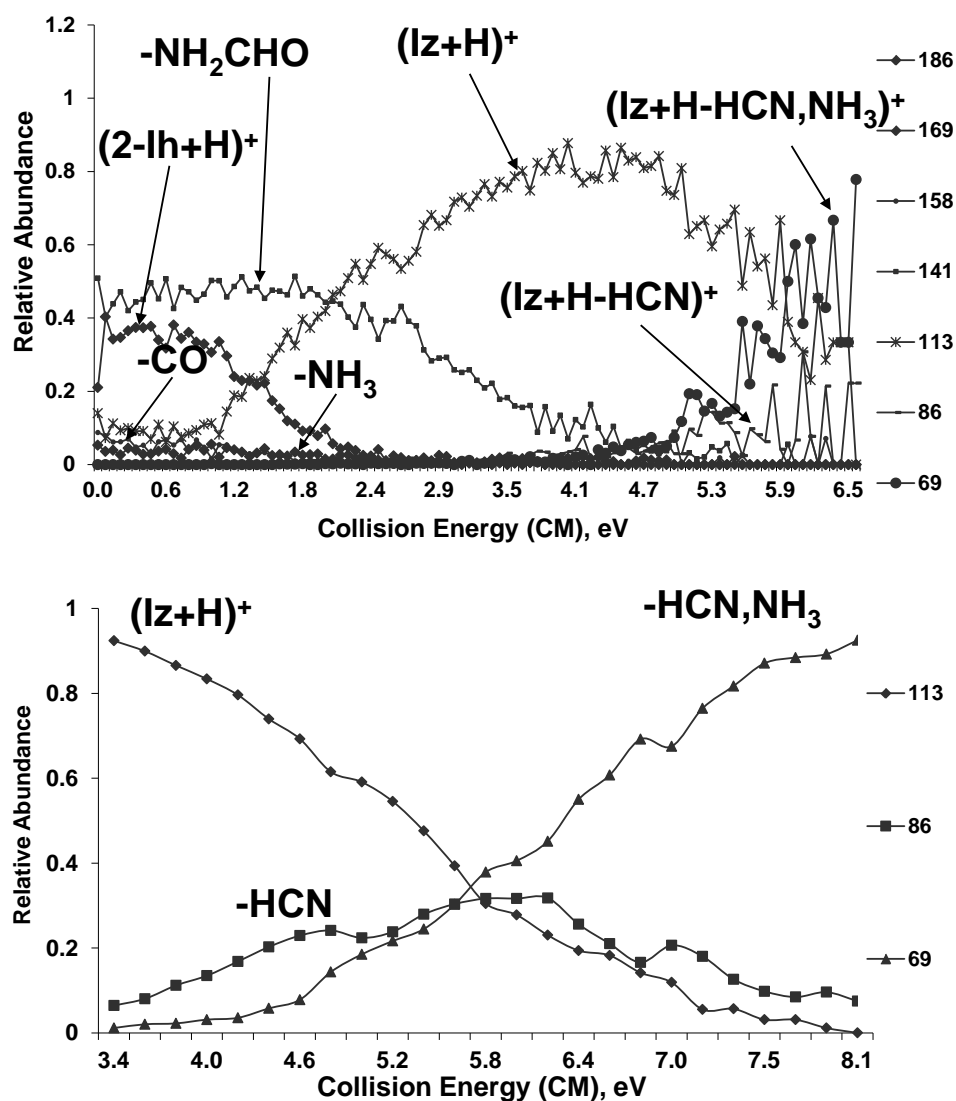


Figure S3. Dissociation profile for the product ions observed in oxidation of guanine by hydrogen peroxide: $(2-lh+H)^+$ (top) and $(lz+H)^+$ (bottom). The loss of NH_2CHO in $(2-lh+H)^+$ was further explored by H-D exchange, it was found to contain only two exchangeable hydrogens and was thus assigned as NH_2CHO rather than NH_3+CO , both of which are observed as minor losses, but have different origin.

