

A Structural Study of Dithizone Coordination Chemistry

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Electronic Supplementary Information

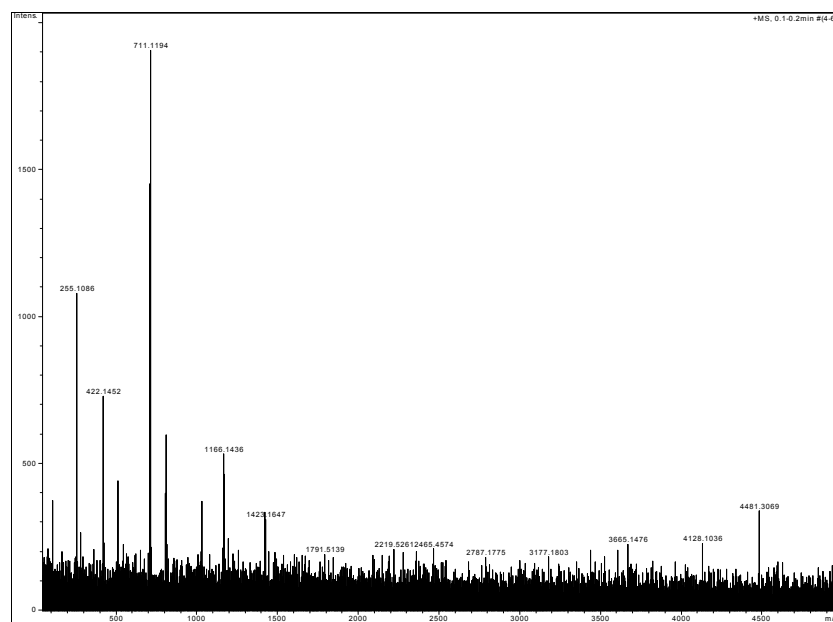


Fig 1. ESI-MS of $[(\text{H-DPTC})_2\text{Hg}]$ showing an ion at m/z 711 corresponding to $[(\text{H}_2\text{-DPTC})(\text{H-DPTC})\text{Hg}]$. Higher mass numbers possibly arise for aggregation in the ESI-MS e.g. m/z 1423 corresponds to $[(\text{H}_2\text{-DPTC})(\text{H-DPTC})_3\text{Hg}_2]$.

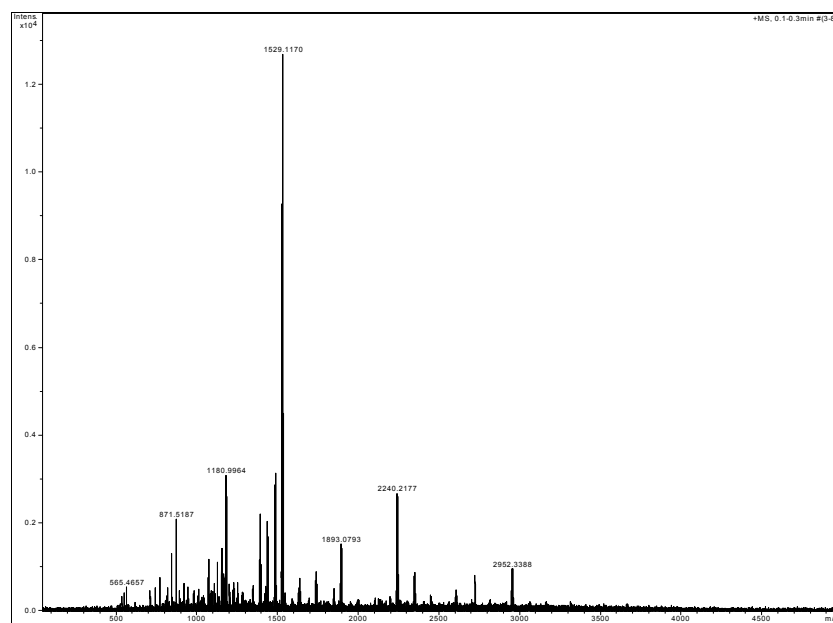


Fig 2. ESI-MS showed ions at m/z 1529 corresponding to $\{[(\text{H-DPTC})_2\text{Hg}]_2\text{Ag}\}^+$ and a small ion at m/z 1737 corresponding to $\{[(\text{H-DPTC})_2\text{Hg}]_2\text{Ag}_2(\text{ClO}_4)]^+$. Again the higher mass numbers possibly arise for aggregation in the ESI-MS e.g. m/z 2240 corresponds to $\{[(\text{H-DPTC})_2\text{Hg}]_3\text{Ag}\}^+$.

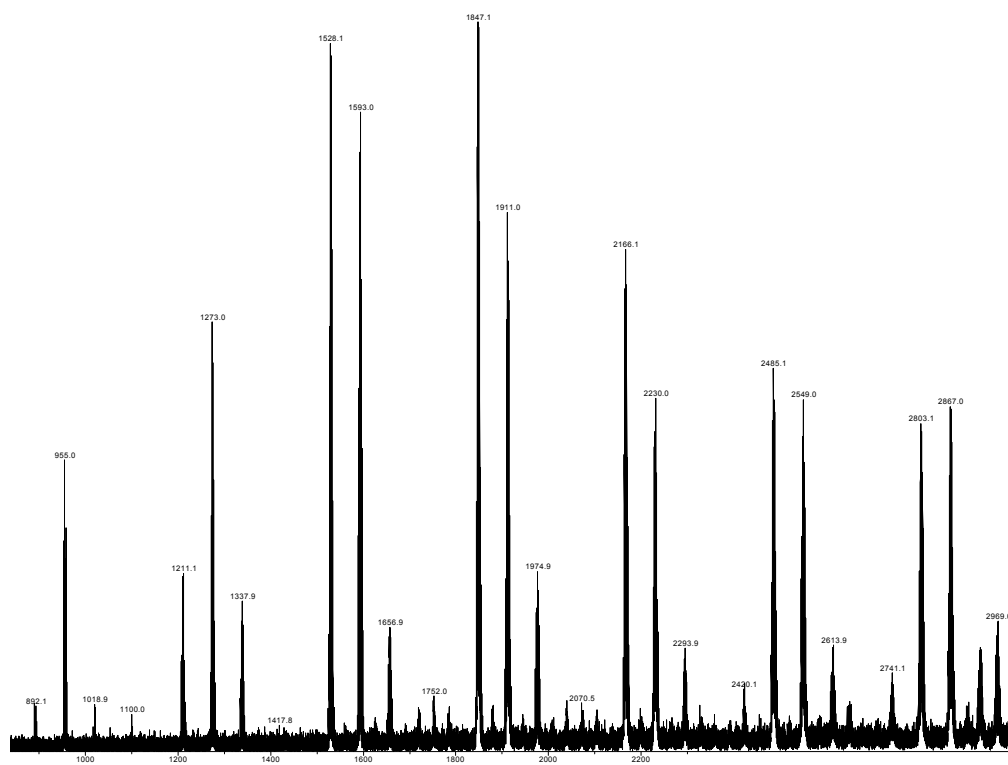


Fig 3. ESI-MS of $[(\text{H-DPTC})_8\text{Cu}_8]$ showing clusters of three ions $\{[(\text{H-DPTC})_n\text{Cu}_{n-1}], [(\text{H-DPTC})_n\text{Cu}_n]$ and $[(\text{H-DPTC})_n\text{Cu}_{n+1}]\}$ where $n = 3 - 9$, including an ion at m/z 2550 corresponding to $\{(\text{H-DPTC})_8\text{Cu}_8\}$. The presence of ions corresponding to $n = 3 - 7$ and $n = 9$.

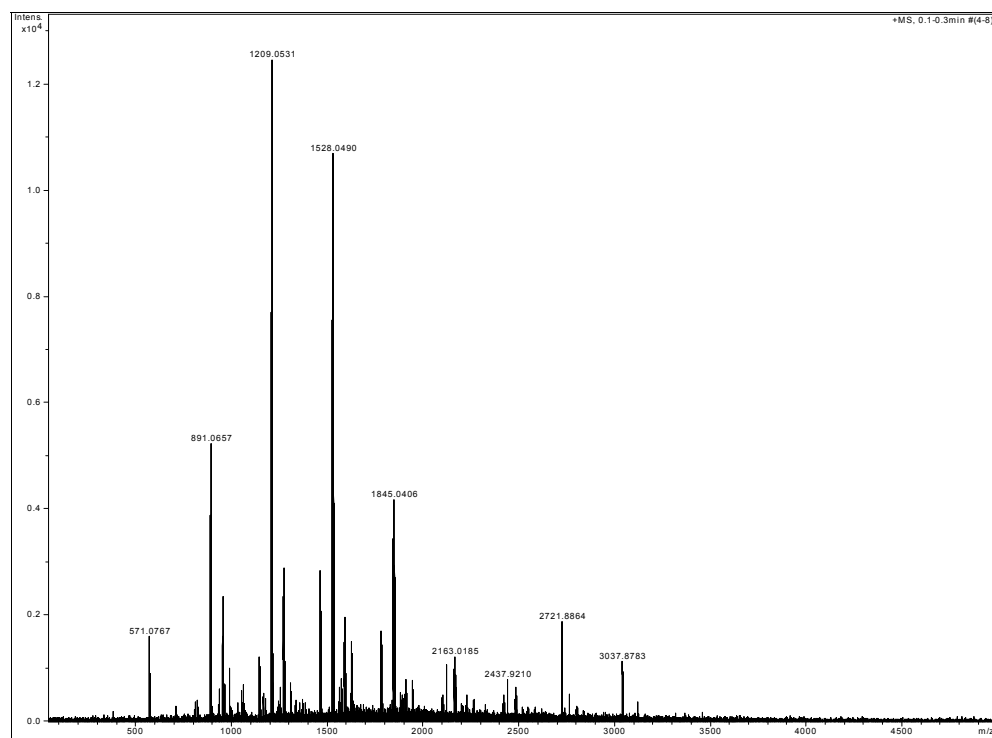


Fig 4. ESI-MS the reaction of DPTC with $\text{Cu}(\text{acetate})_2$ with an ion at m/z 891 corresponding to $[(\text{H-DPTC})_2(\text{DPTC})\text{Cu}_2]$. The higher ions in the ESI-MS e.g. 1209, 1528 and 1845 correspond to $[(\text{H-DPTC})(\text{DPTC})_3\text{Cu}_3]$, $[(\text{H-DPTC})(\text{DPTC})_4\text{Cu}_4]$ and $[(\text{H-DPTC})(\text{DPTC})_5\text{Cu}_5]$. It is probable that this indicates that $\{(\text{H-DPTC})_n\text{Cu}_n\}$ is present in solution or possible aggregation in the ESI-MS.