A Structural Study of Dithizone Coordination Chemistry

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Electronic Supplementary Information

Fig 1. ESI-MS of 
\[(H2-DPTC)_2Hg\] showing an ion at \(m/z\) 711 corresponding to \[(H2-DPTC)(H-DPTC)Hg\]. Higher mass numbers possibly arise for aggregation in the ESI-MS e.g. \(m/z\) 1423 corresponds to \[(H2-DPTC)(H-DPTC)_2Hg_2\].

Fig 2. ESI-MS showed ions at \(m/z\) 1529 corresponding to \{\[(H-DPTC)_2Hg)_2Ag\}^+\ and a small ion at \(m/z\) 1737 corresponding to \{\[(H-DPTC)_2Hg)_2Ag_2(ClO_4)\}^+. Again the higher mass numbers possibly arise for aggregation in the ESI-MS e.g. \(m/z\) 2240 corresponds to \{\[(H-DPTC)_2Hg)_2Ag\}^+. 

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

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