Suggested Structure for $HFeCo_3(CO)_{12}$ and $HRuCo_3(CO)_{12}$

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THE preparation and properties of the anion $FeCo_3(CO)_{12}^-$ and of $HFeCo_3(CO)_{12}$ have been reported by Chini *et al.*[1] We have prepared the complex $HRuCo_3(CO)_{12}$ from $Ru_3(CO)_{12}$ and $Co_2(CO)_8$, by a similar route. This air-stable complex is the first tetrahedral metal-atom cluster in which transition metals from different periods are bonded together.

We believe that the infrared and mass spectra of the two hydride complexes support a structure in which the hydrogen atom is located *inside* the metal-atom cage (I). The evidence on which this conclusion is based is as follows:

Infrared Spectra

(i) The infrared spectra of the anion and hydride are almost identical, suggesting that the two species have the same symmetry. In the anion the peaks are shifted slightly towards longer wavelengths.

(ii) The spectra are also closely similar to that of $Co_4(CO)_{12}$[2] having the same number of carbonyl peaks in both terminal and bridging regions.

(iii) The spectrum of $DFeCo_3(CO)_{12}$ is identical with that of the hydride between 2500 and 800 cm.$^{-1}$ and there is thus no peak which can be assigned to a metal–hydrogen stretching frequency.

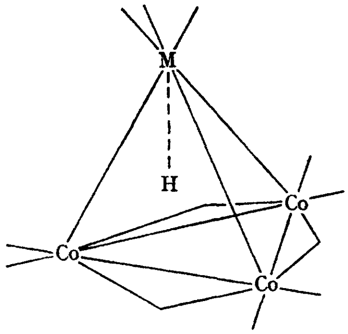
Mass Spectra

(i) No loss of hydrogen is observed from ions of the type $HMCo_3(CO)_n^+$ ($M = Fe, Ru$; $n = 12$—6). A careful analysis of the intensities of the lowest six multiplets ($n = 5$—0) shows that a small percentage of hydrogen loss is occurring from these. In species containing terminal hydrogen atoms [$HMn(CO)_5$] hydrogen loss competes effectively with carbonyl loss from all ions.[3]

(ii) When the tetrahedron fragments, loss of hydrogen becomes an important process and, *e.g.*, $RuCo_2^+$ is of greater intensity than $HRuCo_2^+$.

(iii) Ions containing hydrogen and cobalt only (HCo_3^+, HCo_2^+) are observed in both spectra.

While none of the above evidence is by itself conclusive we believe that the sum total is best accounted for by our suggested structure in which the hydrogen atom, while still formally bonded to iron (or ruthenium), can also interact with the three cobalt atoms. If the metal–metal distance in the tetrahedron is taken as 2·55 Å [Co–Co in $Co_4(CO)_{12}$ = 2·5 Å[4]; Fe–Fe in $Fe_4(CO)_{13}^-$ = 2·6 Å[5]], then placing a hydrogen atom at the centroid gives an average metal–hydrogen distance of 1·5(6) Å, which is not inconsistent with known metal-hydrogen bond lengths.[6]



(I)M=Fe,Ru(carbonyls omitted)

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