# A bonding model for noble gas hydrides and noble gas-noble metal halides

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Dative or/and electron-shared bonding for the H-Ng bond?

$$Ng\text{-}M^{+}\ :X^{-} \leftrightarrow Ng:\ M\text{-}X$$

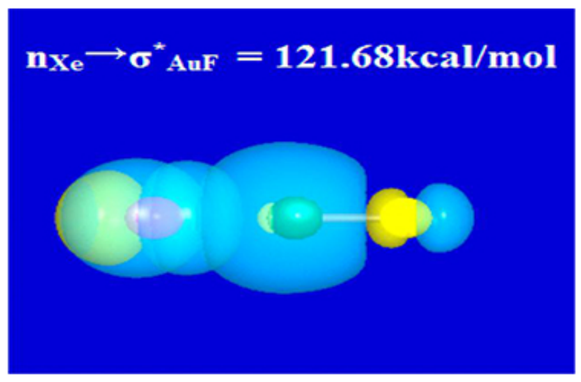


Fig.1 ω-bonding picture of NgMX molecules (Ng=Cu, Ag, Au; X= F, Cl, Br, I).

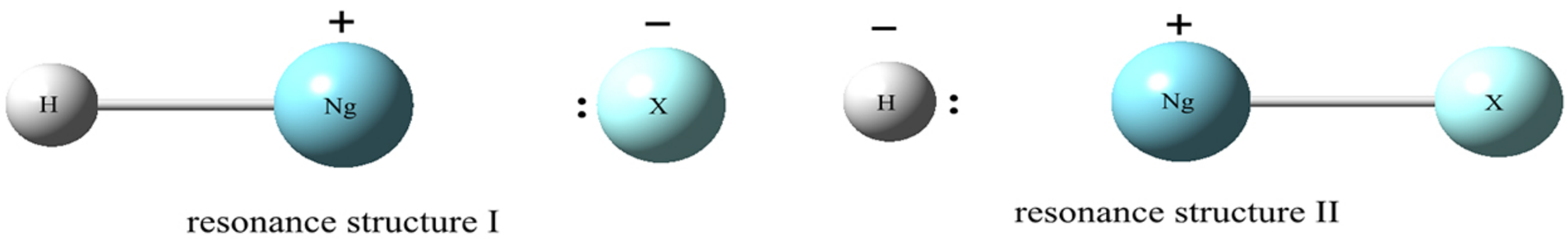


Fig.2 ω-bonding picture of HNgX molecules (Ng=Ne, Ar, Kr, Xe; X= F, Cl, Br, I).

| complexes | $H:^{-}Ng^{+}\text{-}Y$ | $H\text{-}Ng^{+}:Y^{-}$ | X^Y |
|---|---|---|---|
| HXeI | 9.52% | 66.41% | 24.07% |
| HXeI $H_2O$ | 20.33% | 61.63% | 18.05% |
| HXeI HCl | 17.18% | 59.43% | 21.43% |
| HXeI HBr | 19.91% | 59.04% | 18.40% |
| HXeI HI | 20.04% | 58.41% | 18.57% |
| HXeI HCCH | 21.62% | 58.81% | 19.34% |

Tab.1 Resonance weightings of HXeI...HX complexes (HX=$H_2O$, HCl, HBr, HI, HCCH).

Further calculated analyses on the H-Xe blue shift in HXeX…H2O complexes, unexpected add strong evidence to support the duality of dative and electron-shared bonding.The bonding in both HNgX and NgMX molecules is ω-bonding, and that its covalent character is duality of dative and electron-shared bonding. Overall, the present work provides electronic and chemical insights that helps understanding the bonding in these two types of molecules and develop ω-bonding model.