Weakly Coordinating Ligands: Nuclear Quadrupole Coupling Constants and Asymmetry Parameters of Iodocarbons Coordinated to Metal Ions

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NQR (nuclear quadrupole resonance) spectroscopy is potentially one of the best ways of characterizing the bonding of metal cations such as zirconocene cations and Ag^+ to halogen donor atoms in weakly coordinating anions and neutral ligands such as halocarbons. Known coordination of organoiodine atoms to silver ions was studied by ^{127}I NQR spectroscopy in $[Ag(p\text{-}C_6H_4I_2)](PO_2F_2)$, $[Ag(o\text{-}C_6H_4I_2)]NO_3$, $[Ag(CH_2I_2)_2]PF_6$, and the explosive $[Ag(CH_2I_2)]NO_3$; a possible case of iodocarbon coordination to a mercury atom in $C_5Cl_5HgCl\cdot CH_2I_2$ was also investigated. Both the low-frequency (*ca*. 300 MHz) and the high-frequency (*ca*. 500 MHz) NQR signals were detected for each compound, and, for the first time, the quadrupole coupling constants e^2Qq_{zz}/h and asymmetry parameters η of coordinated organohalogen atoms were obtained. As compared to the free iodocarbons, substantial (4 - 12%) reductions of e^2Qq_{zz}/h and substantial increases in η (to about 20 - 40%) were found in the iodocarbon complexes of silver, but not of mercury. From approximate theoretical analysis of the data, it appears that the electronic interaction of silver and iodine is quite substantial.

Key words: Nuclear Quadrupole Interaction; ^{127}I NQR; Asymmetry Parameter; Weakly Coordinating Ligands; Iodocarbon Complexes.