I-129 and Au-197 Mössbauer Spectroscopy of AuI and AgAuI,

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Mössbauer spectroscopy of 129 I and 197 Au nuclei has been applied for AuI and AgAuI₂ to clarify the electronic structures of the gold and iodine atoms, and to investigate the nature of the Au-I bonds. In the 129 I Mössbauer spectra the sign of e^2qQ is positive for AuI, whereas the sign is negative for AgAuI₂. This is attributable to the difference in molecular structures: The iodine atom in AuI is bridged by two gold atoms and in AgAuI₂ the iodine is terminal. The 197 Au Mössbauer spectra suggest that the Au-I bond in AgAuI₂ is more covalent than that in AuI. We have revealed that AgAuI₂ consists of Ag⁺ and linear [I-Au-I]⁻ units from the Rietveld refinement of the X-ray powder diffraction pattern.

Key words: ¹²⁹I Mössbauer Spectra; ¹⁹⁷Au Mössbauer Spectra; Rietveld Analysis; Electric Field Gradient; Isomer Shift.