INSIGHTS INTO THE RARE GAS-SILVER HALIDE INTERACTION FROM A ROTATIONAL SPECTROSCOPIC AND $AB\ INITIO$ STUDY OF XeAgF AND XeAgCl

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XeAgF and XeAgCl have been prepared by laser ablation of Ag metal in the presence of xenon and SF_6, or xenon and Cl_2, respectively. Rotational spectra for 12 isotopomers of XeAgF and 16 isotopomers of XeAgCl have been recorded. Analysis of the spectra indicates that (i) both molecules are unusually strongly bound compared to what is normally found for van der Waals complexes (ii) significant charge rearrangement occurs at the xenon nucleus upon formation of both XeAgF and XeAgCl, as shown by the nuclear quadrupole coupling constant, eQq, of the ^{131}Xe nucleus, and (iii) in both XeAgF and XeAgCl the Xe-Ag distance is small compared to the sum of the Xe van der Waals radius and the Ag^+ ionic radius. An $ab\ initio$ study of the two species has been performed. The nature of the noble gas - noble metal interaction will be discussed.