XENON-COPPER CHEMICAL BONDING: FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF XeCuCl

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High resolution Fourier transform microwave (FTMW) spectroscopy has permitted for the first measurement and characterization of 8 isotopomers of XeCuCl. The molecules were prepared by laser ablation of a Cu metal rod with a pulsed Nd:YAG laser in the presence of Xe and Cl_2 precursors in an Ar carrier gas. The molecules produced in the nozzle were expanded into the spectrometer cavity and stabilized in the supersonic jet. The spectral analysis yielded the rotational and centrifugal distortion constants along with nuclear quadrupole coupling constants for Cu, Cl and ^{131}Xe. The Xe-Cu bond in XeCuCl is short and rigid, and is inconsistent with van der Waals bonding. The nuclear quadrupole coupling constants indicate considerable rearrangement of electron density on complex formation. Ab initio calculations support the experimental findings. All evidence, both experimental and theoretical, is consistent with covalent bonding between Xe and Cu in XeCuCl.

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