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Covalency in Actinide and Lanthanide Hexachloride Anions PING YANG, ENRIQUE BATISTA, RICHARD MARTIN, Los Alamos National Laboratory, CHRISTIN CARLSON, DAVID CLARK, STEVEN CONRADSON, DANIEL SCHWARZ, MARINNE WILKERSON, Seaborg Institute, Los Alamos National Laboratory — Whether actinide atoms form covalent or ionic bonds is still a matter of debate after many years of study and it remains a challenge for experimentalists and theoreticians. From the experimental side, synchrotron-based ligand K-edge X-ray absorption spectroscopy appears as a promising technique for probing this issue. From the theoretical perspective, quantum chemical simulations should be able to add on a first principle understanding. To tackle this problem, we have applied these techniques on a series of octahedral uranium and lanthanide chloride salts, MCl_6^{n-} (M= U, Ce, Pr) in various oxidation states (n=1, 2, 3). We will show hybrid density functional theory calculations that give evidence of the covalent nature of the M-Cl bond in a quantitative manner. This covalency was found to increase for higher oxidation states.

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