Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Structure and Bonding in Crystalline Cesium Uranyl Tetrachloride under Pressure

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I. Electron density study

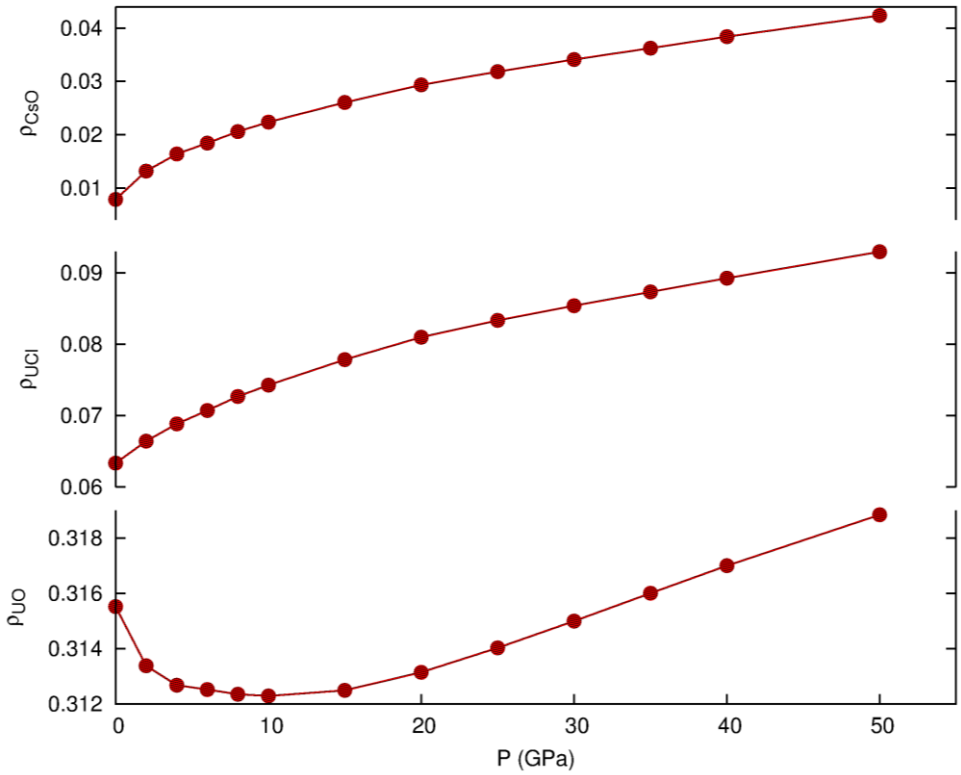

Figure S1. Electron density (e/bohr^3) at the critical bond points at several pressures.

II. Electronic structure calculations in a model system

Computational Details

Cluster calculations were performed using the Gaussian09 code with two functionals, B3LYP (hybrid) and PBE (GGA), Dunning augmented double-z basis were used for Cs, O and Cl atoms. For U atoms a 60 electron pseudopotential was used in combination with a double-z basis.
A grid of U-Cl and U-Cs fixed distances was made. U-Cl distances ranged from 2.4 to 2.8 A in steps of 0.01 A and U-Cs distances ranged from 4.0 to 5.5 A in steps of 0.02 A. The rest of the internal coordinates were optimized for each point of the grid.

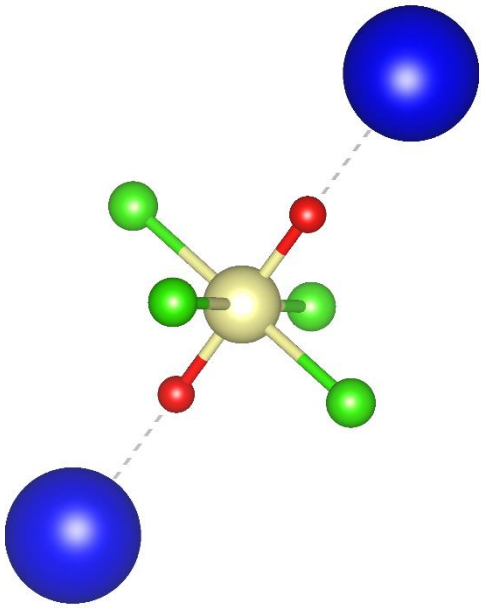

Figure S2. A representation of the model system (U = yellow, O = red, Cl = green, Cs = blue).

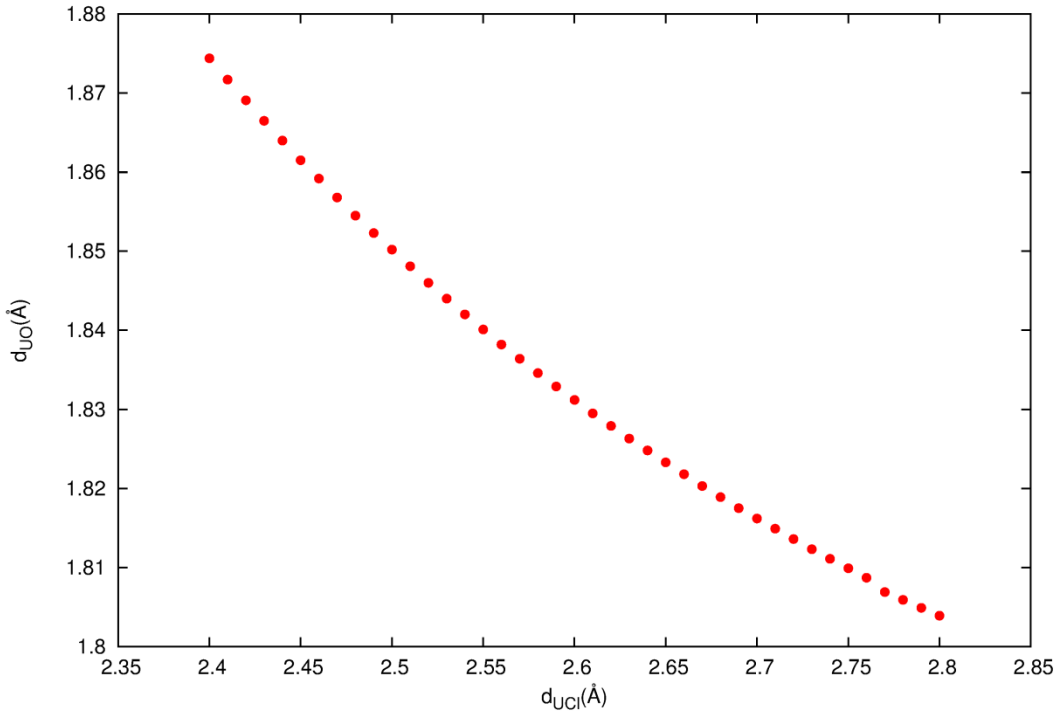

Figure S3. U-O vs U-Cl distances obtained in the cluster calculations (U-Cs fixed at 5.1 Å)

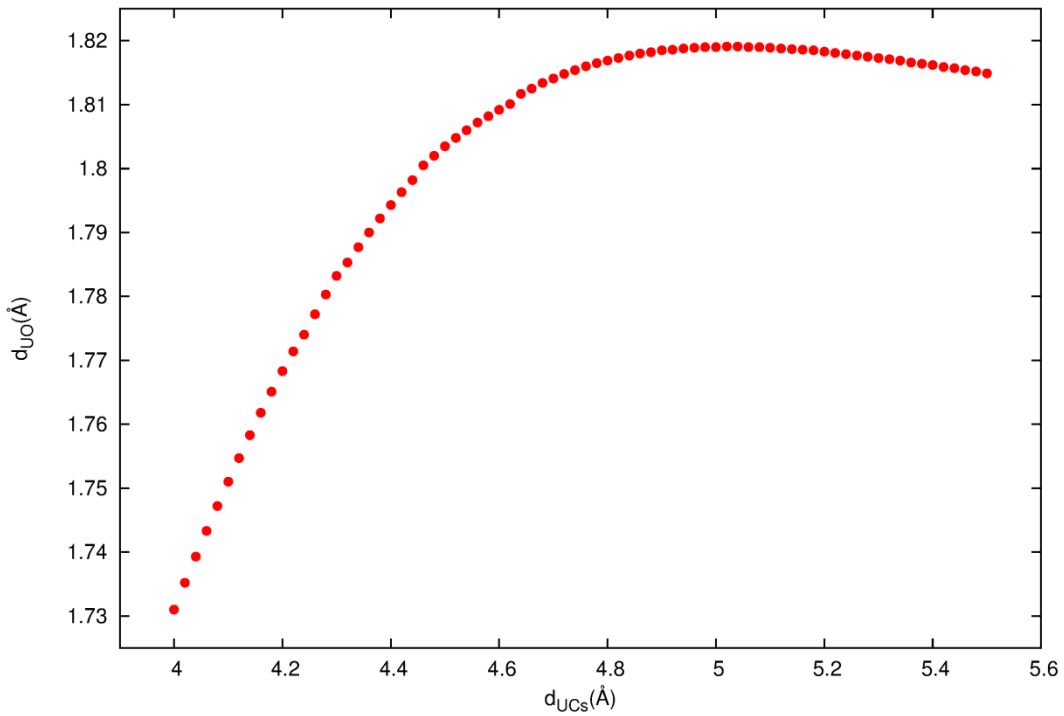

Figure S4. U-O vs U-Cs distances obtained in the cluster calculations (U-Cl fixed at 2.68 Å)

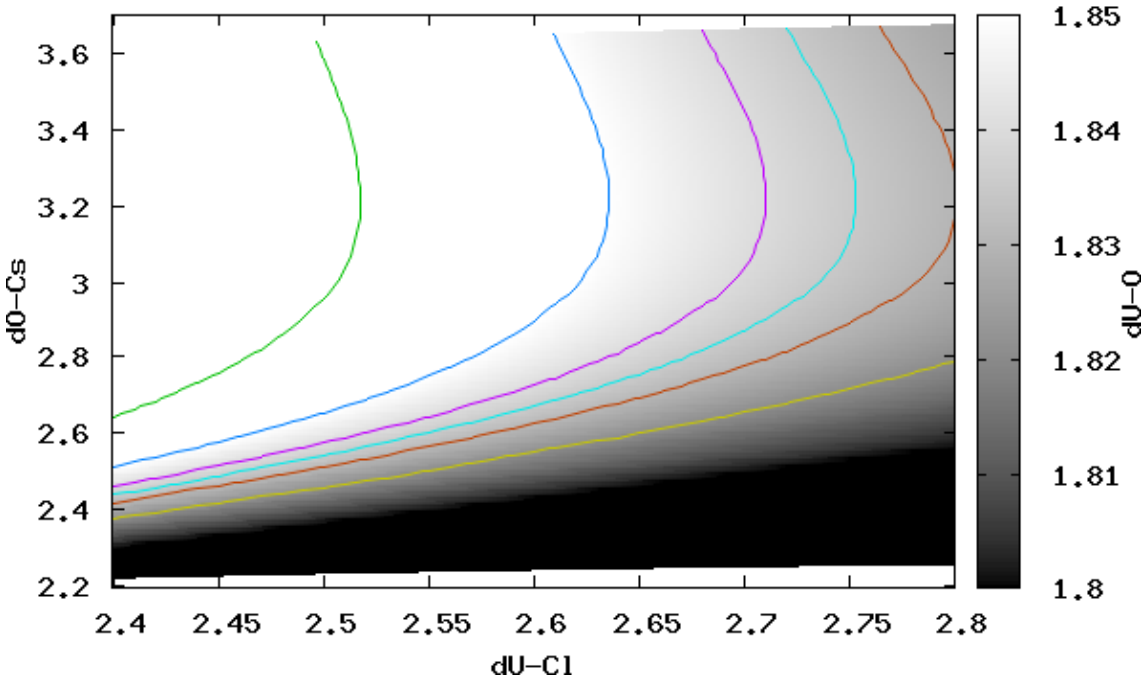

Figure S5. Contour lines and color mapping of U-O distance versus U-Cl and O-Cs distances, obtained in the cluster calculations (PBE functional)

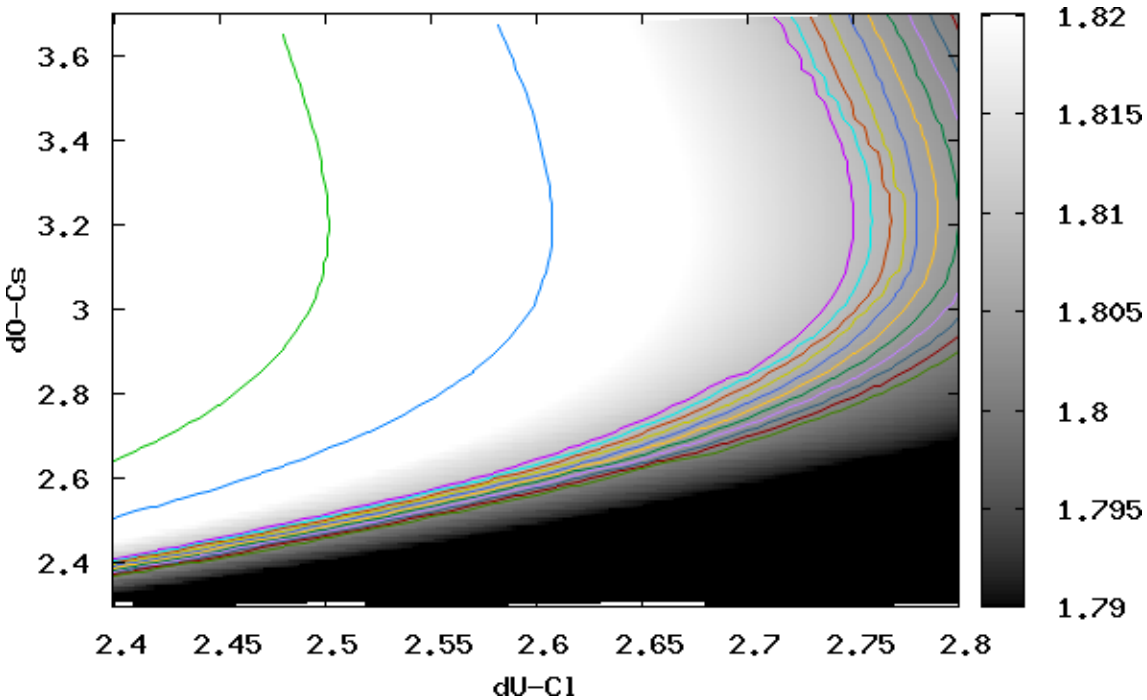

Figure S6. Contour lines and color mapping of U-O distance versus U-Cl and O-Cs distances, obtained in the cluster calculations (B3LYP functional)