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ELECTRONIC SUPPLEMENTARY INFORMATION

Coordination core of Ag(I) N-heterocyclyc carbene (NHC) complexes with anticancer properties as revealed by Synchrotron Radiation X-Ray Absorption Spectroscopy

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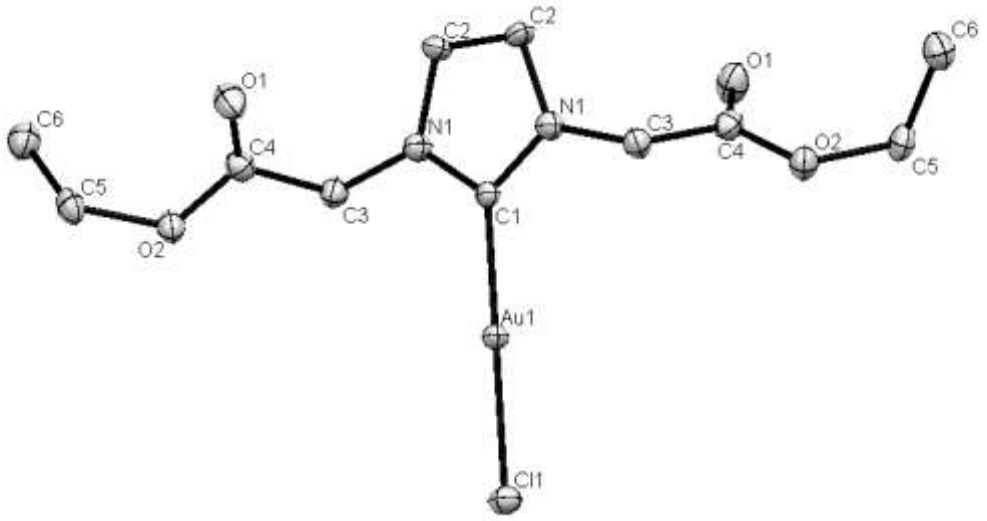

Figure S1. Partial ORTEP structure for complex 1. Hydrogen atoms have been removed due to the its low scattering power which lead to negligible contribution for the electron scattering in EXAFS. Full information on this structure is available on Ref. 21.

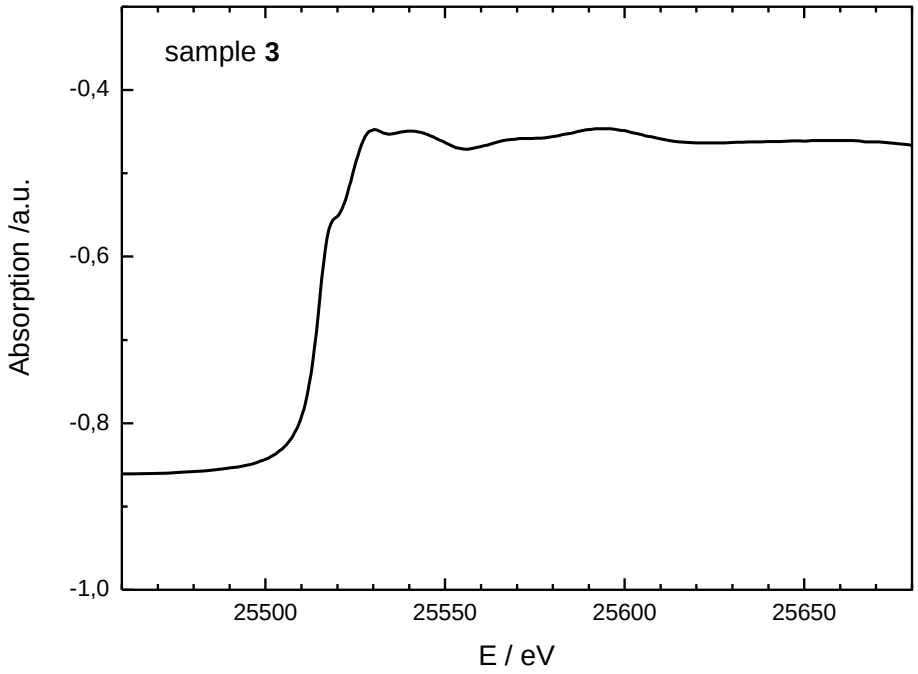

Figure S2. Ag K-edge XANES spectrum of complex 3.

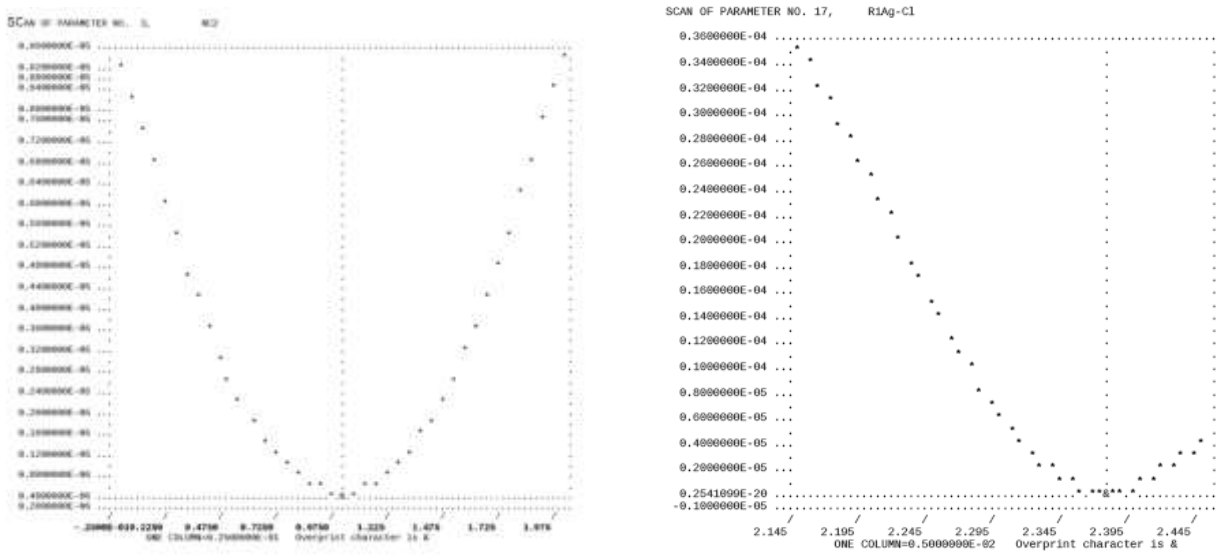

Figure S3: Tests of the EXAFS fitting data for complex 3. The figures displays the fitting index values (to be minimized during the fitting procedure) as a function of the Ag-Cl bond distance (at the right) and as a function of the Ag-Cl relative coordination number (left). The test have been obtained during a scan where all the other parameters were kept fixed to their optimized values. It is clear evident the two regions of minima which identify nearly one Ag-Cl interaction at about 2.39 Å. Also, it is noteworthy the large increase of the fitting index when the CN approaches zero.

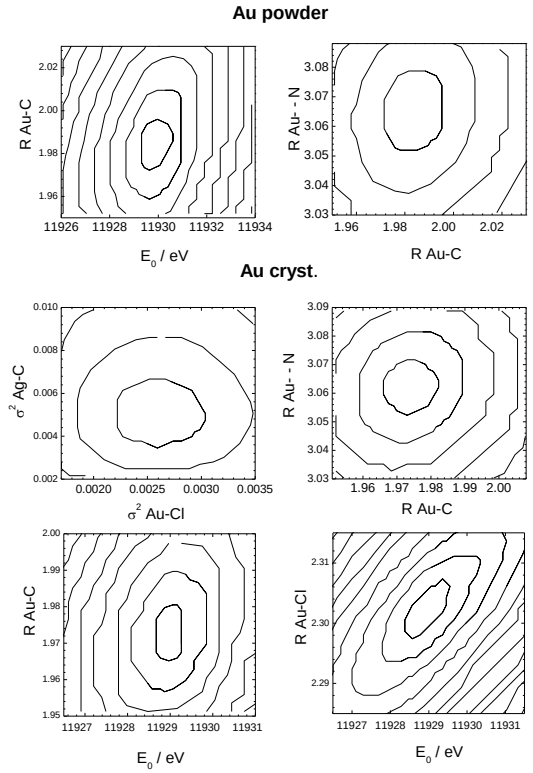

Figure S4: Contour plots. Two dimensional section of the parameter space (contour plots) for complex 2. These plots were selected among the parameters having strong correlation to reflect the highest error. The inner elliptical contour corresponds to the 95% confidence level.

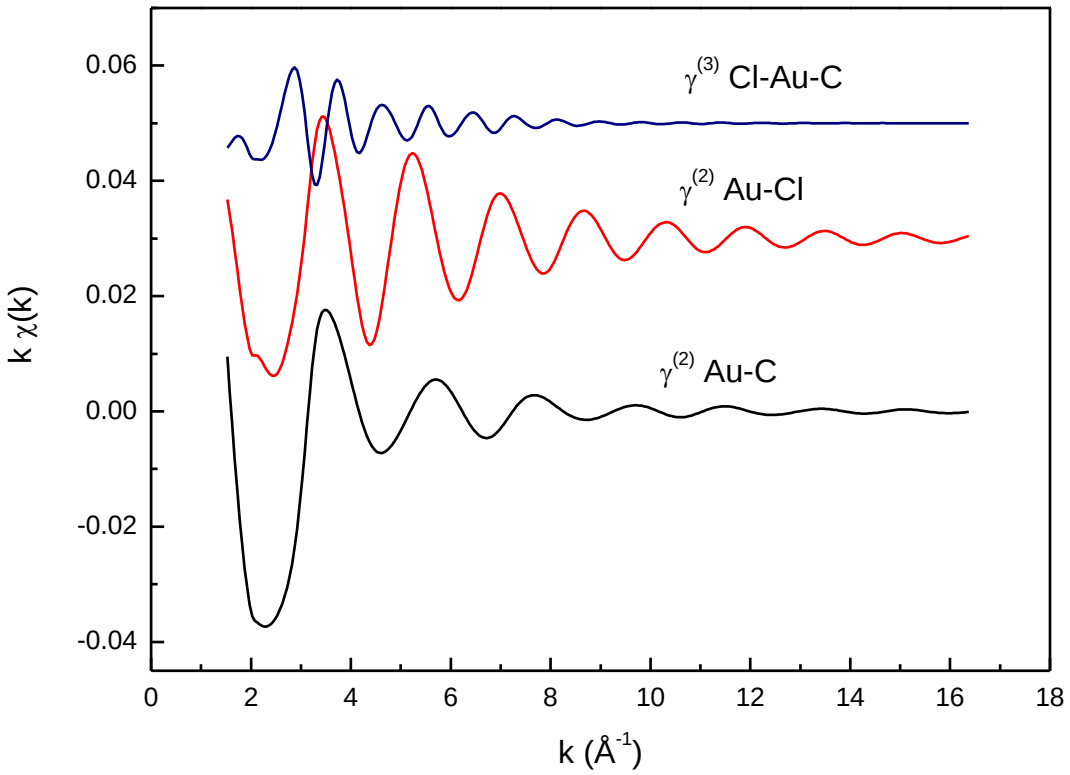

Figure S5: Theoretical signals obtained by *ab-initio* calculation for the gold complex **1**, using the atomic coordinated reported in the reference 21. The Au-C and Au-Cl two-body contributions are the most intense signals, also modulating the entire spectrum. The Cl-Au-C three body multiple scattering (MS) term appears to be negligible in comparison to the other two two-body signals. This is confirmed by taking into account that damping factors has not yet been applied. Therefore the Cl-Au-C three body signal has not been considered in the fitting procedure. The overall path length of the Cl-Au-C triplet is 4.27 Å, considering the planar Cl-Au-C angle and Au-Cl and Au-C distances of 2.28 and 1.99 Å, respectively. This contribution would have been outside the range described by the experimental FT curve of Figure 2, if included in the fitting analysis.