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Relativistic Hirshfeld atom refinement of an organo-gold(I) compound

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During the last 50 years, relativistic quantum chemistry has undergone significant developments and methodological progress. Nowadays, it is well-known that a relativistic quantum formalism is necessary for the study of compounds with heavy elements1-3.
Within last years it has appeared that quantum crystallography is a very prospective method of refinement of crystal structures. It relies on the high-resolution and high-quality XRD data to describe crystal structure in unprecedented details4-5. Intensities of the diffracted beam are affected not only by relativistic effects but also by many other effects such as absorption6, anharmonic motion7, anomalous dispersion8, and others effects which significantly influence electron density distribution in the crystal and, in consequence, derived properties.
In this study, we validated relativistic Hirshfeld atom refinement (HAR)9 as implemented in Tonto10 by performing refinement of experimental high-resolution X-ray diffraction data for an organo-gold(I) compound. The influence of relativistic effects on statistical parameters, geometries and electron density properties was analyzed and compared to the influence of electron correlation and anharmonic atomic motions.

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