

## Charge density study of halogen-halogen interactions in Palladium(II) complex

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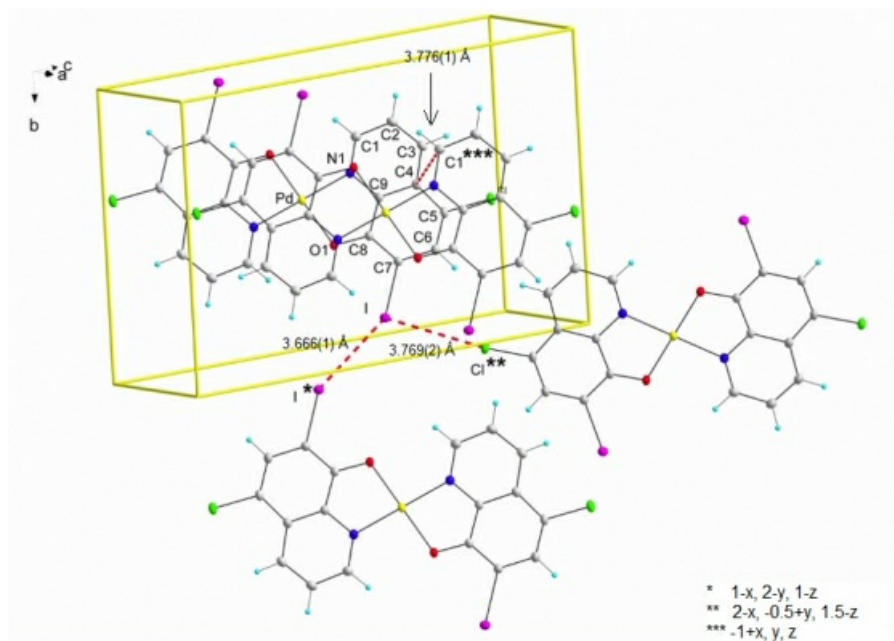
The studied [Pd(CQ)<sub>2</sub>] complex (1) (CQ = clioquinol (5-chloro-7-iodo-quinolin-8-ol)) was prepared as potential anticancer agent. Monocrystal X-ray structure analysis revealed that the palladium atom in the studied complex is coordinated by two pairs of nitrogen and oxygen atoms from two coplanar molecules of CQ in trans positions. Very low solubility of (1) in the polar or non-polar solvents was ascribed to the presence of nonbonding n-n interactions. In addition, halogen-halogen interactions known from the literature were assumed. To prove such interactions, additional charge density studies of (1) were performed.

Data collection was performed on a Stoe STADIVARI diffractometer with a Dectris Pilatus 300K detector and with an Incoatec  $\mu$ S Ag microfocus source (Ag-K $\alpha$ ,  $\lambda = 0.56083 \text{ \AA}$ ) at 100 K using a nitrogen gas open-flow cooler Cobra from Oxford Cryosystems. Data reduction was processed using X-Area (Stoe, 2016). For numerical absorption corrections a crystal-shape model with 8 faces was employed. An average redundancy of 10.4 gives Rint of 4.34%. Direction cosines were applied for the anisotropic secondary extinction correction. The results of multipole refinement were performed on F<sub>2</sub> using XD suite of programs. After the multipole refinement a topological analysis of the charge density was done. Halogen-halogen interactions were compared with the literature. There are known values for iodine-iodine interaction in solid iodine, for F•••F intermolecular interaction and for Cl•••Cl interaction, which are comparable with values obtained from (1).

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