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BOOK OF ABSTRACTS

CHALCOGEN BONDING INVOLVING SQUARE PLANAR PLATINUM(II) COMPLEXES BEARING CHELATING LIGANDS

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Noncovalent interactions play an important role in many advanced areas of modern science ranging from polymer chemistry to molecular biology. While amount of studies on hydrogen bonding, halogen bonding, and metallophilic interactions involving metal centers is gradually increased, many novel types of noncovalent forces including, e.g., metal-involving chalcogen bonding were recognized only recently thus providing a new tool for crystal engineering [1].

Square-planar transition metal complexes bearing sterically available d_{z^2}-orbitals are the most suitable objects for constructing supramolecular systems via noncovalent interactions involving metal centers [2,3]. In this work, two new platinum(II) complexes with chelating ligands, viz. [Pt(PPy)($S_2CN(CH_2)_n$)] (PPy – 2-phenylpyridine; n = 4 (**1**), 6 (**2**)), were synthesized. The complexes were co-crystallized with chalcogen bond donors, namely bis(perfluoropyridyl) telluride $(FPy)_2Te$ and bis(perfluorotolyl) telluride $(FTol)_2Te$, to give three new cocrystals – **1**·$(FPy)_2Te$, **2**·$(FPy)_2Te$, and **2**·$(FTol)_2Te$, respectively. The structures of the obtained adducts were studied by single-crystal X-ray diffraction (XRD; Fig. 1).

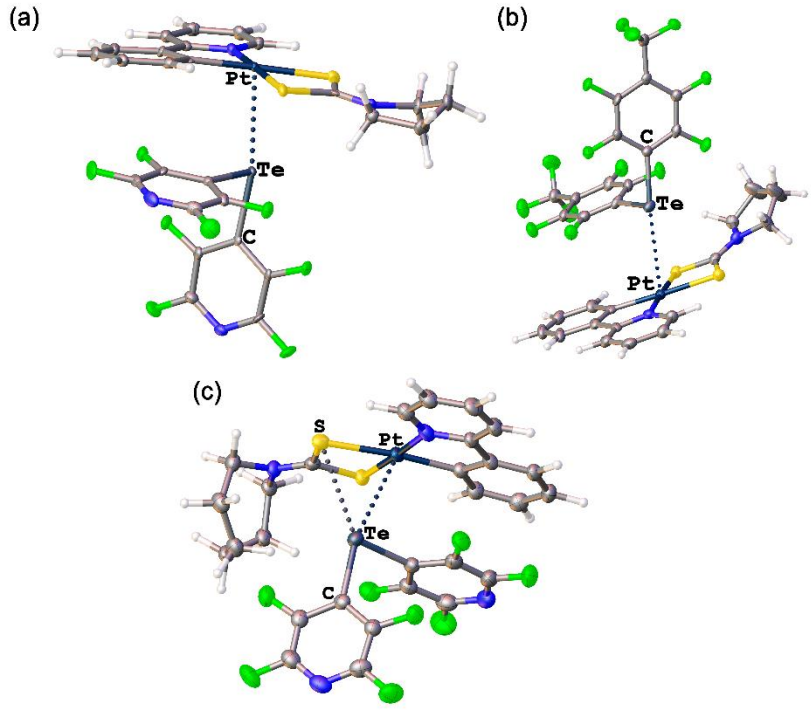

Figure 1. Metal-involving chalcogen bonds in cocrystals: (a) **2**·$(FPy)_2Te$, (b) **2**·$(FTol)_2Te$, and (c) **1**·$(FPy)_2Te$.

Upon analysis of noncovalent interactions in the XRD structures of the cocrystals, we identified various types of intermolecular contacts. In addition to previously known π-π stacking, LP(F)···π, and Te···S interactions, we found rare metal-involving Te···Pt^{II} chalcogen bonds (Fig. 1a and 1b) and recognized hitherto unknown bifurcated (μ_2-Te)···[Pt^{II},S] contacts (Fig. 1c). The noncovalent nature of the revealed interactions was confirmed theoretically by DFT calculations via several computational tools.

References

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[2] *Inorg. Chem. Front.* **2022**, *9*, 2869
[3] *Inorg. Chem. Front.* **2021**, *8(10)*, 2505