

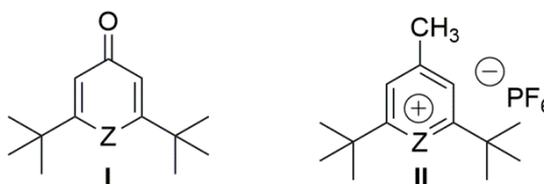
## Crystal Structure of the Chalcogen-Containing Precursors for Polymethine Dyes

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Polymethine dyes are potential materials for all-optical signal processing.<sup>1</sup> However, in order for these materials to retain their favorable solution properties in the high-number density films, their molecular aggregation should be reduced. To limit aggregation, bulky groups may be introduced in several positions of the dye to protect the  $\pi$ -conjugated system from interacting with itself.<sup>2,3</sup>

Currently, we are presenting the investigation of thio-, seleno- and telluro-pyranones and chalcogenopyrylium salts with bulky *tert*-butyl groups, which were prepared as described previously.<sup>4</sup> The general scheme of studied compounds is presented below, where Z is S, Se, or Te.



The crystal structures of thio- and seleno-pyranones **I** atoms are isostructural and crystallize in P2<sub>1</sub>/c space group. There are no any special intermolecular contacts in these crystals. However, introduction of larger Te atom in telluro-pyranone changes the crystal structure, and it contains hydrogen-bonded dimers with H...O distance 2.58 Å.

The crystal structures of seleno- and telluropirylium salts **II** are isomorphous and crystallize in C2/c space group. Both structures contain three symmetrically independent cations and three PF<sub>6</sub><sup>-</sup> anions. In crystal, the molecules form hexamers containing two of each symmetrically independent molecules connected by six PF<sub>6</sub><sup>-</sup> anions. The hexamers are packed in columns along [0 0 1] direction. Our research provides an insight into the crystal structure and intermolecular interactions that may occur in polymethine dyes.

### References

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