

## Luminescence properties of the antifungal agent ketoconazole and its diphenylphosphane derivatives.

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### Streszczenie

In this paper we present a physico-chemical characterization of ketoconazole (**Ke**) and four derivatives: diphenylphosphane (**KeP**), where acetyl group is replaced with  $-\text{CH}_2\text{PPh}_2$  moiety and the phosphane chalcogenides: oxide (**KeOP**), sulphide (**KeSP**) and selenide (**KeSeP**). The antifungal activity of these compounds was recently studied, showing that they are promising antifungal agents towards *Saccharomyces cerevisiae* and *Candida albicans*. All the compounds share the same mode of action, which is to inhibit the cytochrome P450 14 $\alpha$ -demethylase. However, differences in antifungal activity suggest that there may be additional modes of action or important interactions with other cellular components. The further understanding of the action mechanisms of these compounds will demand a detailed study of their interactions with different potential molecular partners, and understand their behavior in different molecular environments. Therefore, in this study we characterized thoroughly the luminescence characteristics of **Ke**, as well as of its diphenylphosphano derivatives using fluorescence spectroscopy techniques and DFT calculations. It has been shown that their main absorption and luminescence bands, which result from a mixture of  $\pi \rightarrow \pi^*$  and  $n \rightarrow \pi^*$  transitions located at the  $-1,3\text{-dioxolan-4-yl-C}_6\text{H}_4\text{-}$  piperazine aromatic ring, overlap the transitions at the  $-\text{CH}_2\text{P(X)Ph}_2$  moiety which thereby acts as a intramolecular fluorescence quencher.

### Słowa kluczowe

Ketoconazole, Phosphanes, Luminescence, DFT, Molecular modeling

### Adres publiczny

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