The FDA requires that the absolute stereochemistry of any chiral drugs be determined for regulatory submission. However, chiral compounds may often prove to be the most desirable drug candidate. Thus reliable methods for establishing the absolute stereochemistry of these candidates are essential within the pharmaceutical industry. It has been known for many years that the absolute stereochemistry of structures can be determined by a single crystal X-ray diffraction anomalous dispersion experiment [1]. For structures containing atoms heavier than sulphur this process is fairly straightforward and can be carried out on a standard laboratory Mo Kα diffractometer. However, for structures consisting only of light atoms the process can prove more complex. In the work presented the use of single crystal x-ray diffraction for establishing the absolute structure of both light and heavy atoms will be discussed. This will include the use of the well-known Flack parameter [2] and a new method created by Hooft, Straver and Spek for determining the absolute structure of chiral compounds based on the Bijovet pair intensity differences and accessible via the program Platon [3].

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MS21 O4

Crystallochemical, vibrational and optic Studies of the silver doped $NaY(PO_3)_4$ structure. M. El Masloumi[a], (b), V. Jubéra[a], S. Pechev[a], J. P. Chaminade[a], J. J. Videau[a], M. Mesnaoui[b], M. Maazaz[b], B. Moine[c].
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Keywords : Crystal structure ; Phosphate ; Silver luminescence ; decay time

Since ten years, the study of the optical properties of monovalent silver phosphates was undertaken by the LCSM of Marrakech (Morocco) in collaboration with the ICMCB (France), these investigations related to the well crystallize materials as vitreous [2]. It made it possible to identify three centers of luminescence covering the whole of the visible one.
The aim of this work is, on the one hand, to widen the range of the compositions crystallized in order to facilitate a deepening of the comprehension of the mechanisms of luminescence of the various types of association of the ions Ag^+ while optimizing the output of photoluminescence and on the other hand, to associate the silver ions rare earth in new phosphates (crystals and glasses), in seen to examine their mutual influences (creation of new centers, transfer of energy between centers, interaction between silver clusters and ions rare earth, etc.) and to understand the mechanisms of them.
It is in this context that the structure $NaY(PO_3)_4$ in single-crystal form, could be established by diffraction of X-rays (**$P2_1/n$**).This phase will enrich the family by the metaphosphate of general formula $NaLn(PO_3)_4$ (**Ln = La**[3]**, Nd, Gd, Er**).A comparative study of the influence of rare earths on the structure could be carried out and interpreted.
In parallel, the study of luminescence carried out on crystals of composition $Na_{0.9}Ag_{0.1}Y(PO_3)_4$ showed two types of emission. Measurements of declines of luminescence make it possible to advance mechanisms of fluorescence of the silver

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A boron based antifungal agent in complex with its target protein domain

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Aminoacyl-transfer RNA (tRNA) synthetases, which catalyze the attachment of the correct amino acid to its corresponding tRNA during translation of the genetic code, are proven antimicrobial drug targets.
Recently, we showed that the broad-spectrum antifungal 5-fluoro-1,3-dihydro-1-hydroxy-2,1-benzoxaborole (AN2690), which is in development for the treatment of onychomycosis and inhibits the fungal leucyl-tRNA synthetase (LeuRS), also binds to bacterial LeuRS by formation of a stable LeuRS-AN2690 adduct in the editing site of the enzyme. Adduct formation is mediated through the boron atom of AN2690 and the 2'- and 3'-oxygen atoms of tRNA's3'-terminal adenosine. The trapping of enzyme-bound tRNA in the LeuRS editing site prevents catalytic turnover, thus inhibiting synthesis of leucyl-tRNA and consequentially blocking protein synthesis [1].
We now present x-ray structures of a fungal LeuRS editing domain, the real drug target, alone and in complex with a similar adduct. Together with our low resolution x-ray structure of the human LeuRS editing domain (3.1 Å) and homology modeling results, these data open the way for rational drug improvement.

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