

## Electronic Structure of $\text{Tl}_3\text{PbI}_5$ , a Prospective Nonlinear Optical Material

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The first appearance of the  $\text{Tl}_3\text{PbI}_5$  compound was detected when studying the pseudo-binary  $\text{TlI}-\text{PbI}_2$  system [1]. It was found that  $\text{Tl}_3\text{PbI}_5$  melts congruently at 639 K. Olekseyuk et al. [2] have discovered that  $\text{Tl}_3\text{PbI}_5$  crystallizes in the orthorhombic (space group  $\text{P}2_12_12_1$ )  $\text{Tl}_3\text{PbBr}_5$ -type structure, with the lattice parameters:  $a = 16.205 \text{ \AA}$ ,  $b = 9.676 \text{ \AA}$ , and  $c = 8.952 \text{ \AA}$ .

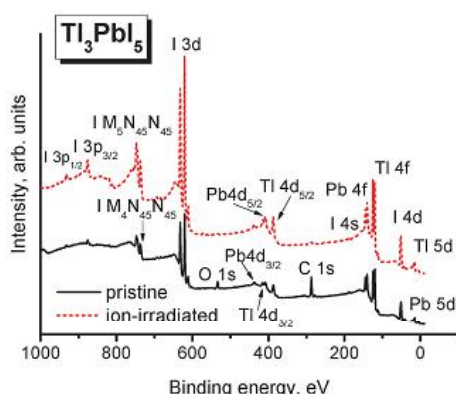


Fig. 1 Survey XPS spectra recorded for a pristine (solid line) and  $\text{Ar}^+$ -ionbombarded (dashed line) surface of the  $\text{Tl}_3\text{PbI}_5$  single crystal

Fig. 1 presents the survey XPS spectra of the pristine and  $\text{Ar}^+$ -ion irradiated surfaces of the  $\text{Tl}_3\text{PbI}_5$  single crystal. It is apparent that all the spectral features, except for the carbon and oxygen 1s levels for a pristine surface, are assigned to be the constituent element core-levels or Auger lines. Fig. 1 shows that the relative intensity of the C 1s core-level line for the pristine  $\text{Tl}_3\text{PbI}_5$  single crystal surface was found to be rather weak, and the line almost completely vanishes after the  $\text{Ar}^+$  ionbombardment of the surface. As can be seen from Fig. 1, the present survey XPS data show that there is no active chemical interaction with oxygen when the  $\text{Tl}_3\text{PbI}_5$  single crystal surface is exposed to air for comparatively long time (about 1 month): the O 1s line is rather weak on the studied pristine surface and no trace of the O 1s line is detected after the  $\text{Ar}^+$  ion-bombardment of the surface. Therefore, our XPS results reveal the low hygroscopicity of  $\text{Tl}_3\text{PbI}_5$ , the property that is very important for handling this compound as an efficient laser source operating in ambient conditions.

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2. I. D. Olekseyuk, G. E. Davidyuk, A. A. Fedonyuk, L. V. Sysa and A. M. Padalko, *Inorg. Mater.*, 1998, 34, 445.