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**Radiative defects in thallium chacolgenide semiconductors**[1] J.A. PETERS, N.K. CHO, ZHIFU LIU, B.W. WESSELS, Dept. of Materials Science and Engineering, Northwestern University, S. JOHNSEN, S. NGUYEN, M. SEBASTIAN, M.G. KANATZIDIS, Dept. of Chemistry, Northwestern University, Evanston, IL 60208 — Thallium chalcohalides constitute a promising new class of semiconductor compounds for radiation detectors. Due to their wide energy bandgap, high atomic number, and high resistivity, they are being considered as potential replacement for conventional II-VI semiconductor x-ray and $\gamma$-ray detectors for room temperature operation. For these applications resistivities of $\sim 10^{10}$ ohm-cm are required. Although defects play a major role in detector response, little is known about their nature and origin in these compounds. We have investigated $Tl_6I_4Se$ and $Tl_6I_4S$ compounds which have bandgaps of 1.86 and 2.03 eV, respectively. Photoluminescence (PL) spectra of single crystals were investigated in the 650-885 nm wavelength region and over a temperature range of 20-100 K. For $Tl_6I_4Se$ we observed PL bands centered at 1.61 eV. A detailed study of the peak, as function of temperature and excitation intensity, indicates that it is due to radiative transitions from donor-acceptor pairs (DAP). The ionization energies of the donor and acceptor levels in $Tl_6I_4Se$ were estimated at 52 and 290 meV, respectively. Similarly DAP emission in $Tl_6I_4S$ with a peak at 1.66 eV was observed. The role of crystalline stoichiometry in DAP formation is currently under study.

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