

Abstract Submitted  
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**Stoichiometry Driven Impurity Configurations in Compound Semiconductors**<sup>1</sup> G. CHEN, I. MIOTKOWSKI, S. RODRIGUEZ, A. K. RAMDAS, Purdue University — Precise stoichiometry and departures therefrom in the composition of the tetrahedrally coordinated compound semiconductors allow impurity incorporation in more than one configuration. Ultra-high resolution infrared spectroscopy of CdTe:O at low temperatures reveals a unique pair of sharp lines, a non-degenerate  $\nu_1 = 1096.78 \text{ cm}^{-1}$  and a doubly degenerate  $\nu_2 = 1108.35 \text{ cm}^{-1}$  at 5 K, associated with the local vibrational modes of  $O_{Te}$  in a  $(O_{Te} - V_{Cd})$  complex in crystals grown with  $(\text{CdTe} + \text{CdO} + \text{excess Te})$  or  $(\text{CdTe} + \text{TeO}_2)$  which enhances the occurrence of Cd vacancy ( $V_{Cd}$ ); in contrast, a single, triply degenerate sharp line at  $\nu_0 = 349.79 \text{ cm}^{-1}$  observed at 5 K occurs in CdTe grown with  $(\text{CdTe} + \text{CdO} + \text{excess Cd})$  in which the appearance of  $V_{Cd}$  is inhibited. In the former, oxygen,  $O_{Te}$ , is bonded to three nearest neighbor Cd's with a nearby  $V_{Cd}$ . The latter corresponds to  $O_{Te}$  attached to all the four nearest neighbor Cd cations. With increasing temperature,  $\nu_1$  and  $\nu_2$  approach each other and behave as a single triply degenerate line at  $\nu_0^*$  for temperature  $T \geq T^* \sim 300 \text{ K}$ ; the uniaxial ( $C_{3v}$ ) symmetry of  $(O_{Te} - V_{Cd})$  transforms to  $T_d$  symmetry at  $T^*$ , acquired due to an increasing rate of bond switching among the four possible  $O_{Te} - V_{Cd}$  directions as  $T$  approaches  $T^*$ .

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