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**X-ray and *ab initio* Molecular Structures for a Series of Mixed Valence Species.** Tiffany Kinnibrugh,<sup>c</sup> Stephen Barlow,<sup>ab</sup> Chad Risko,<sup>a</sup> Veaceslav Coropceanu,<sup>a</sup> Simon C. Jones,<sup>a</sup> Tatiana Timofeeva,<sup>c</sup> Seth Marder,<sup>ab</sup> Jean-Luc Bredas<sup>a</sup>, School of Chemistry & Biochemistry & Center for Organic Photonics & Electronics, Georgia Inst. of Technology, Atlanta GA 30332, Dept. of Chemistry, Univ. of Arizona, Tucson AZ 85721, Dept. of Natural Sciences, New Mexico Highlands, Las Vegas NM 87701.

Several mixed valence species based on triarylamine redox centers, have demonstrated two photon absorption and charge transfer properties. Charge transfer has been of considerable interest for its applications in organic light-emitting diodes. Three different species (neutral **I**, **[I]<sup>+1</sup>SbF<sub>6</sub>**, and **[I]<sup>+2</sup>(SbF<sub>6</sub>)<sub>2</sub>**) of compounds **I** and two different species (neutral **II**, and **[II]<sup>+2</sup>(SbF<sub>6</sub>)<sub>2</sub>**) of compounds **II** were synthesized and their molecular and crystal structures were determined by X-ray diffraction. The X-ray molecular structures were compared with *ab initio* calculations.

