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Magneto-Optic Properties of Small Atomic Clusters of Ga and In with As and V LIUDMILA POZHAR, Western Kentucky University, Department of Chemistry, Bowling Green, KY 42101, ALAN YEATES, FRANK SZMULOWICZ, WILLIAM MITCHEL, Air Force Research Lab, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433 — The magneto-optic properties of small, virtually (i.e., fundamental theory-based, computationally) pre-designed and vacuum pyramidal clusters of Ga-As-V and In-As-V atoms have been investigated by means of the Hartree-Fock (HF) method. The optic transition energies (OTEs) of these clusters are about 3 times smaller than those specific to small Ga-As-P and In-As-P clusters of the same structure and numbers of Ga and In atoms studied earlier. The HF analysis of the spin density distributions for In-based clusters suggests that these clusters possess noticeable magnetic properties: their total spin density distributions (SDDs) expand beyond the space occupied by the cluster's atoms and can be considered as collective features of the entire corresponding clusters, rather than individual atoms. In the case of the Ga-based clusters with V atoms the absolute values of the SDDs are an order of magnitude lesser than those specific to similar In-based clusters. Unfortunately, stabilization of such In-based clusters grown experimentally may involve chemical means, both in vacuum and in confinement.

Liudmila Pozhar
Western Kentucky University, Department of Chemistry
Bowling Green, KY 42101

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