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第一原理計算による硫化ヒ素分子の構造多様性
Ab initio quantum chemical investigation of arsenic sulfide molecular diversity

興野 純 [1*]
Atsushi Kyono[1*]

[1] 筑波大学大学院生命環境系地球進化科学専攻
[1]Div. of Earth Evolution Sci., Grad. Sch. of Life & Environmental Sci., Univ. of Tsukuba

The structural diversity of arsenic sulfide molecules in compositions between As_4S_6 and As_4S was investigated using ab initio quantum chemical calculations. The As_4S_6 molecule consists of four trigonal pyramid coordinations of As atoms bonding to three S atoms. In the As_4S_5 composition, only one type of molecular configuration corresponds to an uzonite-type molecule. In the As_4S_4 composition, two molecular configurations exist with realgar-type and pararealgar-type molecules. Three molecular configurations are in the As_4S_3 composition. The first configuration comprises trigonal pyramidal As atom coordinations of two types: bonding to two S atoms and one As atom, and bonding to one S atom and two As atoms. The second is the molecular configuration of dimorphite. The third comprises trigonal pyramidal As atom coordinations of two types: bonding to three As atoms, and bonding to one As atom and two S atoms. The As_4S_2 composition allows molecular configurations of two types. One is comprised of trigonal pyramidal As atom configurations of one type bonding to two As atoms and one S atom. The other comprises trigonal pyramidal As atom coordinations of three types: bonding to two S atoms and one As atoms, bonding to one S atom and two As atoms, and bonding to three As atoms. The As_4S molecule has trigonal pyramidal As atom coordinations of two types: bonding one S atom and two As atoms, and bonding to three As atoms. The As_4S composition permits only one molecular configuration, which suggests that the mineral duranusite comprises the As_4S molecular geometry. In all, ten molecular configurations are predicted in the molecular hierarchy of the arsenic sulfide binary system. The simulated Raman spectral profiles are helpful in searching for undiscovered arsenic sulfide minerals.
Keywords: arsenic sulfide minerals, molecular configuration, diversity, hierarchy, ab initio quantum chemical calculation