

AB INITIO CHARACTERIZATION OF SULFUR COMPOUNDS AND THEIR CHEMISTRY FOR VENUS AND THE INTERSTELLAR MEDIUM

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The atmosphere of Venus is known to contain trace amounts of SO, SO₂, OCS, H₂SO₄, and possibly H₂S and elemental sulfur oligomers, S_n. Modeling studies indicate that many more compounds containing sulfur and both sulfur and chlorine may also be present, given that the known compounds are photolyzed by solar radiation in the upper atmosphere of Venus and yield reactive radical species. A large number of exotic compounds containing S, O, H, C, and/or Cl of suspected or plausible significance for Venus chemistry have been characterized at the RCCSD(T)/aug-cc-pVTZ level, yielding structures, dipole moments, and dipole polarizabilities. Representative compounds and associated chemical reactions will be discussed. Both abstraction and addition-elimination reactions have been characterized.