MONOBRIDGED Si_2H_4

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The rotational spectrum of a novel monobridged isomer of Si_2H_4, denoted here as $H_2SiHSiH$, has been detected by means of Fourier transform microwave spectroscopy in a supersonic molecular beam through the discharge products of silane. On the basis of high-level coupled cluster theory, this isomer is calculated to lie only 7 kcal/mol above disilene (H_2SiSiH_2), the most stable isomeric arrangement of Si_2H_4, and to be fairly polar, with a calculated dipole moment of $\mu = 1.14$ D. The rotational spectrum of $H_2SiHSiH$ exhibits closely-spaced line doubling, characteristic of a molecule undergoing high-frequency inversion motion; at the CCSD(T) level of theory the barrier height to inversion is calculated to be 10-11 kcal/mol. Because of its favorable energetics and high polarity with respect to either disilene or silylsilylene, monobridged Si_2H_4 is a good candidate for radioastronomical detection in sources such as IRC+10216 where other large silicon-bearing molecules have already been discovered.