Gas-phase structures of dithietane derivatives, including an electron diffraction study of 1,3-dithietane 1,1,3,3-tetraoxide.

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Streszczenie

The gas electron diffraction structure of 1,3-dithietane 1,1,3,3-tetraoxide has been determined using the SARACEN method to restrain parameters that otherwise could not be refined. Quantum chemical calculations for this species showed that the potential-energy surface was extremely flat, and this was also observed from the diffraction experiments. The difference in goodness of fit for the diffraction experiment between a planar ring and one puckered by up to 9° was very small. Calculations were also performed for a variety of similar species with different numbers of oxygen atoms attached to the sulphur atoms. Topological analysis of the electron density, and electron localisation function studies of the relevant molecules, have given deeper insight into the nature of their bonding, and suggested how spatial localisation of electron pairs may influence the molecular structure.

Słowa kluczowe

Gas electron diffraction, Dithietanes, Quantum chemical calculation, SARACEN, AIM theory, Electron localisation function

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