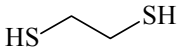
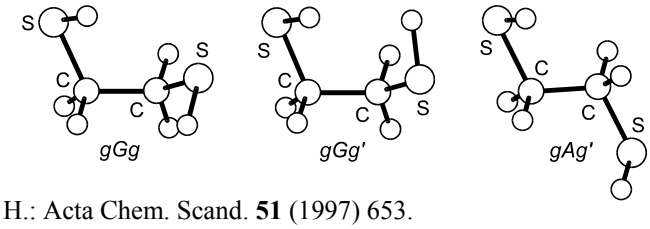
306 **$C_2H_6S_2$** **1,2-Ethanedithiol** **C_2 (*gGg'*)**
MW **C_2 (*gAg'*)**
C_1(*gGg*)



Three conformers were detected: *gGg, gAg'* and *gGg'*. The *gAg'* conformer is 3.2(4) kJ mol^{-1} more stable than *gGg* and 1.8(4) kJ mol^{-1} more stable than *gGg'*. The *gGg* conformer is stabilized by one weak S–H...S intramolecular hydrogen bond, whereas *gGg'* is stabilized by two such bonds. The *gAg'* conformer displays tunneling in the ground vibrational state and in the first excited state of the C–C torsional vibration. The tunneling is presumably caused by a concerted rotation by both thiol groups. The tunneling frequency is 0.575(80) MHz in the ground vibrational state, and 2.48(5) MHz in the first excited state of the C–C torsion. Tunneling is absent in the *gGg* and *gGg'* conformers.



Marstokk, K.-M., Møllendal, H.: Acta Chem. Scand. **51** (1997) 653.

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