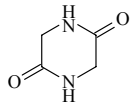
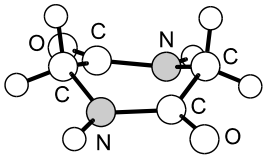
535 **$C_4H_6N_2O_2$** **2,5-Dioxopiperazine** **C_2**
MW 2,5-Piperazinedione
Diketopiperazine



The stable form is a boat configuration having C_2 symmetry (see figure); the "methylene boat" conformer is the only stable conformer. The microwave spectrum deviated from that of a rigid rotor in that all of the measured transitions were members of doublets in which the separation was *ca*. 2 GHz. This is attributed to tunneling between two equivalent conformations through a relatively low barrier on the potential energy surface. *Ab initio* calculations indicate that the minimum energy pathway linking the two boat (C_2) enantiomeric conformers passes over a barrier of about 470 cm^{-1}. The chair (C_i) conformer is involved at the summit of the barrier. This barrier is significantly lower in energy than the planar ring (C_{2h}) species, which appears to be a higher saddle point on the potential energy hypersurface. The calculated energy barrier is plausibly consistent with the tunneling splitting found in the spectrum.



Bettens, F.L., Bettens, R.P.A., Brown, R.D., Godfrey, P.D.: J. Am. Chem. Soc. **122** (2000) 5856.