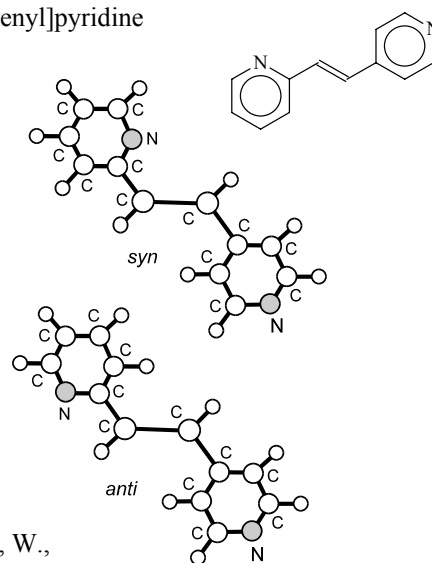


903 **C₁₂H₁₀N₂**
MW, DFT calculations

1-(2-Pyridyl)-2-(4-pyridyl)ethene
2-[(*E*)-2-(4-Pyridinyl)ethenyl]pyridine

C_s

A two-dimensional potential of the pyridyl torsions well reproduces the experimental inertial defect: -1.295 u \AA^2 . Spectra of only one conformer was assigned, and the effect of introducing a weakly binding N...H interaction in the stilbene frame, combined with a simple model based on the DFT calculations, rationalizes the energetics and structural differences of the two conformers of the molecule. According to the results of BLYP/6-31G* calculations, the *syn* conformer is more stable than the *anti* conformer.



Melandri, S., Maccaferri, G., Favero, P.G., Caminati, W.,
Orlandi, G., Zerbetto, F.: J. Chem. Phys. **107** (1997) 1073.