

CONFORMATIONS OF p-METHOXYPHENETHYLAMINE, A NEUROTRANSMITTER

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p-Methoxyphenethylamine ($\text{CH}_3\text{OC}_6\text{H}_4\text{C}_a\text{H}_2\text{C}_b\text{H}_2\text{NH}_2$) is a neurotransmitter. Seven conformers have been identified by electronic spectroscopy¹ and their conformational identities characterized by analogy to simpler related compounds, empirical force field and quantum chemical calculations, and vibrational spectra. With the $\text{C}_a\text{-C}_b$ bond lying in a plane nominally orthogonal to the benzene ring, there are nine possible conformers. With C(phenyl)- $\text{C}_a\text{-C}_b\text{-N}$ gauche, the NH_2 group has 3 possible orientations. These are doubled by the two possible planar orientations of the methoxy group. With C(phenyl)- $\text{C}_a\text{-C}_b\text{-N}$ anti, the NH_2 group again has 3 distinguishable orientations. A pair of the C(phenyl)- $\text{C}_a\text{-C}_b\text{-N}$ gauche conformers with the N lone pair directed toward the benzene ring were deemed to be missing in the electronic spectroscopic studies. The rotational spectrum was investigated at a rotational temperature near 1 K in a pulsed-jet Fourier transform microwave spectrometer. Rotational spectra of four conformers have been assigned with preliminary rotational constant values of 2832.545, 538.362, and 509.172 MHz; 2740.111, 542.176, and 507.522 MHz; 2789.609, 535.220, and 509.950 MHz; and 2750.592, 548.056, and 507.537 MHz. They all correspond to conformers with a C(phenyl)- $\text{C}_a\text{-C}_b\text{-N}$ gauche conformation coupled with the methoxy group "anti" or "syn" to the gauche NH_2 group. Structural characterization is continuing. More lines remain to be assigned.

¹S. J. Martinez III, et al., *J. Molec. Spectrosc.*, 158, 82(1993) and I. Unamuno, et al., *J. Phys. Chem. A*, 104, 4364(2000).