CONFORMATIONS OF p-METHOXYPHENETHYLAMINE, A NEUROTRANSMITTER

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p-Methoxyphenethylamine ($CH_3OC_6H_4C_aH_2C_bH_2NH_2$) is a neurotransmitter. Seven conformers have been identified by electronic spectroscopy[a] and their conformational identities characterized by analogy to simpler related compounds, empirical force field and quantum chemical calculations, and vibrational spectra. With the C_a-C_b bond lying in a plane nominally orthogonal to the benzene ring, there are nine possible conformers. With C(phenyl)-C_a-C_b-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)-C_a-C_b-N anti, the NH_2 group again has 3 distinguishable orientations. A pair of the C(phenyl)-C_a-C_b-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)-C_a-C_b-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.

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