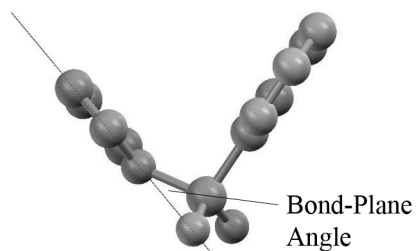


W0537

Bond-Plane Angle in Pyrrole Systems as an Indicator of the Degree of Aromaticity. David A. Grossie, P.G. Seybold, Daniel M. Ketcha, Dept. of Chemistry, Wright State Univ., Dayton, Ohio 45435.



The structures of many 1-benzenesulfonyl pyrroles have been determined in the examination of the regioselectivity of Friedel-Crafts acylations of the pyrrole. In the analysis of the 1-benzenesulfonyl and 1-tosylpyrrole structures, interesting variations in the geometry of the pyrrole nitrogen atom have been noted. The angle between N-S bond and the mean plane of the pyrrole ring varies from 0 to 27.5 degrees in the structures examined, indicating a change in the hybridization in the nitrogen atom. If a condition of aromaticity demands sp^2 hybridized atoms, then this change in the bond-plane angle may be a useful indicator of the degree of aromaticity.