X-RAY DIFFRACTION INVESTIGATION OF SILOXANES. III. STRUCTURE AND CONFIGURATION OF CYCLIC TETRA- AND PENTASILOXANES BEARING DIFFERENT ORGANIC SUBSTITUENTS AT SILICON ATOMS

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Single crystal X-ray diffraction is applied to elucidate the structures of six tetra- and one penta-siloxane compounds differing in the nature and position of silicon-sitting organic substituents (Me — methyl, Ph — phenyl, mPh — methoxyphenyl, 2mPh — dimethoxyphenyl, 3mPh — trimethoxypehnyl, and C_4H_6N — butironitrile). Charge states of atoms in the siloxane molecules are calculated, and the effect of oxygen-containing radicals on the Si–O bond lengths and Si–O–Si bond angles affecting the configurations of the tetra- and pentasiloxane cycles is shown .

Keywords: cyclic siloxanes, organic substituents, interatomic distances, hydrogen bond.