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ortho-Benzene Derivatives with Meshed Cogwheel Chloromethyl and Methylamino Substituents: Structures and Rotation Enthalpy Hypersurfaces

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Facets of molecular dynamics in organic compounds such as coupled rotations of adjacent substituents are advantageously discussed based on structural data. Within this context, crystal structures of spatially overcrowded ortho-disubstituted benzene derivatives with chloromethyl or methylamino groups are presented together with semiempirical enthalpy hypersurfaces for the substituent rotation. Both compounds, 1-trichloromethyl-2-dichloromethyl-benzene as well as 1-trimethylammonium-2-dimethylamino-benzene exhibit comparable steric overcrowding and their preferred dynamics are predicted to be dominated by the rotation of the threefold substituted group during an approximate standstill of the twofold substituted, mirror-symmetric one. According to known solid state NMR measurements as well as to atom/atom-potential model calculations for the pentachloro *ortho*-xylene derivative, this molecular dynamic mode is still active in the crystal.

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