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ortho-Benzene Derivatives with Meshed Cogwheel Trimethylsilyl Substituents: Structural Comparison with Benzene-1,2-disulfonate Salts and Rotation Enthalpy Hypersurfaces

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ortho-Benzene derivatives with adjacent bulky propeller substituents are well-suited model compounds to investigate their potentially coupled rotations. To approach the molecular dynamics of 1,2-bis(trimethylsilyl)benzene, a liquid at room temperature and containing heteroelement substituents, an advantageous starting point are the crystal structures of the stereochemically correspondent benzene-1,2-disulfonate dianion salts. For both the rotations of the synperiplanar three-bladed rotor-groups $-SO_3^{\ominus}$ and $-Si(CH_3)_3$, PM3-enthalpy hypersurfaces are presented, which suggest only weak interdentate interaction and, concomitantly, only partly coupled intermolecular substituent rotation dynamics. Additional data from the Cambridge Structural Database for silicon organic compounds fit into the contour lines of the enthalpy surface calculated for 1,2-bis(trimethylsilyl)benzene, and the structure correlation with varying distances Si···Si between the heteroelement centers can be discussed in more general terms of the substituent propeller blade length *vs.* thickness ratio.

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