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EMPIRICAL AND NOT-SO-EMPIRICAL CORRELATIONS HOLDING FOR ${}^2J({}^{29}\text{Si}-\text{O}-{}^{29}\text{Si})$ COUPLINGS IN INDUSTRIALLY IMPORTANT SILOXANES

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A large number (78) of ${}^2J({}^{29}\text{Si}-\text{O}-{}^{29}\text{Si})$ coupling constants (range 0.4 - 9 Hz) has been determined in siloxanes with different degrees of branching and different substituents. The signs of these couplings were determined for representative model compounds.[1] It was found that all these couplings are positive. In contrast, quantum mechanical calculations (MP2/6-31g** optimized structures, B3LYP/IgloIII J-calculation) yielded negative couplings. Hence our discussion is limited to empirical correlations though some rest on reasonable theoretical bases.

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References

- 1 V. Blechta and J. Schraml, *This conference, Valtice 2011.*