Formation of *meso*-1,2-Bis(dimethylamino)-1,2-diphenylethane by Oxidative C-C Coupling Reaction

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The title compound was obtained from the reaction of *N*,*N*-dimethylbenzylamine with *n*-butyl lithium and sulfur in tetrahydrofuran at room temperature. Its molecular structure was investigated by means of single crystal X-ray diffraction and quantum chemical DFT methods. The formation of *meso*-1,2-bis(dimethylamino)-1,2-diphenylethane is likely to be due to an unusual α-deprotonation of *N*,*N*-dimethylbenzylamine, instead of the well known *ortho*-lithiation, with a subsequent oxidative C-C coupling of the anions. *Ab initio* calculations of the corresponding α- and *o*-deprotonated anions of *N*,*N*-dimethylbenzylamine showed the former to be more stable than the latter, due to delocalisation of the negative charge over the π-system of the phenyl ring. The choice of solvent and temperature is seen as the main reason for the unusual course of the reaction.

Key words: 1,2-Bis(dimethylamino)-1,2-Diphenylethane, C-C Coupling, Crystal Structure, *ab initio* Calculation