9,12-Dithiol-1,2-dicarba-*closo*-dodecaborane as building block for ligands for surfaces, nanoparticles and metal complexes

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Thiolated derivatives of 1,2-dicarba-*closo*-dodecaborane (1,2-$C_2B_{10}H_{12}$) have been used as building blocks with relatively robust icosahedral molecular architecture, and dipole moment (≈3–4 D) for self-assembled monolayers (SAMs) on metal films and nanaparticles,[1, 2] or as ligands for transition metal complexes.[3] 9,12-dithiol-1,2-dicarba-closo-dodecaborane (9,12-$(SH)_2$-1,2-$C_2B_{10}H_{10}$) **1**, a derivative with two SH groups attached to boron atoms at positions 9 and 12 of the ortho-carborane skeleton, is an interesting precursor for the preparation of derivatives additionally functionalized at positions 1 and 2.[4]

A synthetic pathway to 1,2-disubsituted 9,12-dithiolated *ortho*-carboranes has not been reported in the literature so far. In this contribution we show the preparation of 9,12-di(methoxy-methylthio)-*ortho*-carborane **2** (figure 1) as a way of protecting the SH groups against the experimental conditions necessary for introducing additional substituents at positions 1 and 2 via lithiation (structures **3** and **4**).

We have explored the potential of this novel synthetic strategy for the preparation of multi-functionalized ligands suitable for the preparation of new materials derived from self-assembled monolayers (SAMs) on metal films, or nanoparticles and from transition metal complexes.

References

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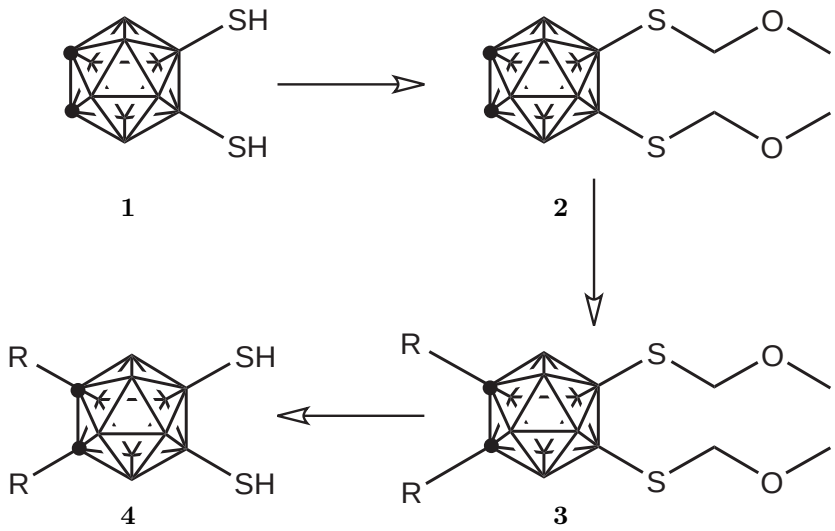

Figure 1: Three step synthesis of 1,2-disubstituted 9,12-dithiolated *ortho*-carboranes: 1) protection of SH-groups using MOM-groups 2) substitution in position 1 and 2 of the carborane icosahedron 3) deprotection of the SH-groups. Black dots in carborane skeleton indicate the carbon atoms.