

Synthesis and characterization of new fluorescent styrene-containing carborane derivatives: the singular quenching role of a phenyl substituent.

A. Ferrer-Ugalde, E. J. Juarez-Perez, F. Teixidor, C. Vinas, R. Sillanpää, E. Perez-Inestrosa, R. Nunez

Chem. Eur. J. **2012**, *18*, 544-553.

Abstract: A set of neutral and anionic carborane derivatives in which the styrenyl fragment is introduced as a fluorophore group has been successfully synthesized and characterized. The reaction of the monolithium salts of 1-Ph-1,2-C₂B₁₀H₁₁, 1-Me-1,2-C₂B₁₀H₁₁ and 1,2-C₂B₁₀H₁₂ with one equivalent of 4-vinylbenzyl chloride leads to the formation of compounds 1–3, whereas the reaction of the dilithium salt of 1,2-C₂B₁₀H₁₂ with two equivalents of 4-vinylbenzyl chloride gives disubstituted compound 4. The closo clusters were degraded using the classical method, KOH in EtOH, to afford the corresponding nido species, which were isolated as tetramethylammonium salts. The crystal structure of the four closo compounds 1–4 were analyzed by X-ray diffraction. All compounds, except 1, display emission properties, with quantum yields dependent on the nature of the cluster (closo or nido) and the substituent on the second C cluster atom. In general, closo compounds 2–4 exhibit high fluorescence emission, whereas the presence of a nido cluster produces a decrease of the emission intensity. The presence of a phenyl group bonded to the C cluster results in an excellent electron acceptor unit that produces a quenching of the fluorescence. DFT calculations have confirmed the charge-separation state in 1 to explain the quenching of the fluorescence and the key role of the carboranyl fragment in this luminescent process.

Keywords: carboranes · cluster compounds · density functional calculations · photoluminescence · styrene

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ejjuarezperez@unizar.es (Emilio)