Semi-empirical modelling of ferrocenyl-containing pyridylphenylene dendrimers

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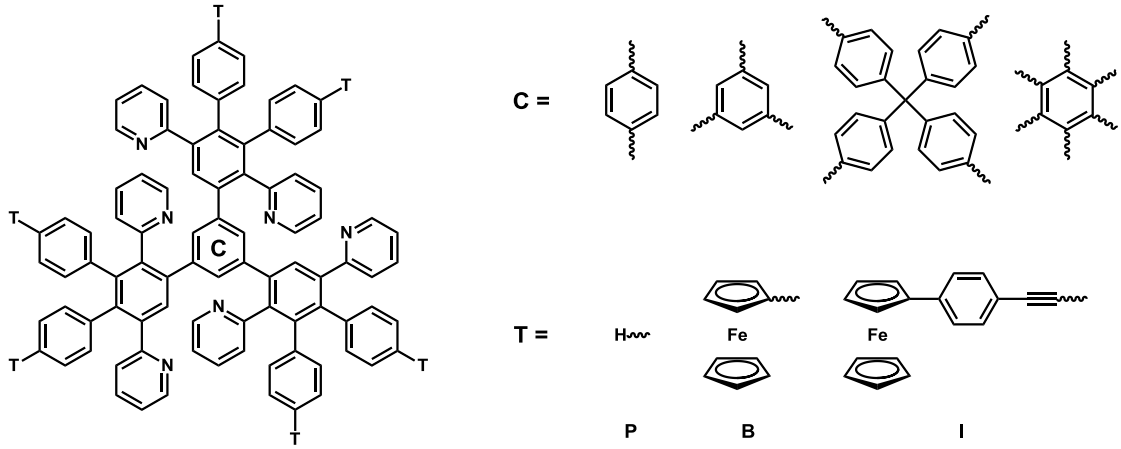
The dendrimer chemistry allows one to obtain monomolecular macromolecules with concise shapes and diverse functionality. In this work, we focused on rigid pyridylphenylene dendrimers augmented with ferrocenyl peripheral groups. Those dendrimers may find various applications in redox catalysis, as electrochemical biosensors or molecular batteries.

The representative example of the first-generation dendrimers is shown in Scheme 1. We optimized (MOPAC, PM7[1]) geometries of 33 similar molecules of 1-3 generations with four different cores (**C**) and three different terminal groups (**T**).



Scheme 1. *General structure of the first-generation dendrimers.*

The dendrimers exhibit various shapes like flat sheets, propellers, tetrahedrons and 3D stars (Figure 1). The typical collision diameter is 1-6 nm. Some dendrimers possess π-stacking interactions between branches that decrease sphericity of the whole molecule.

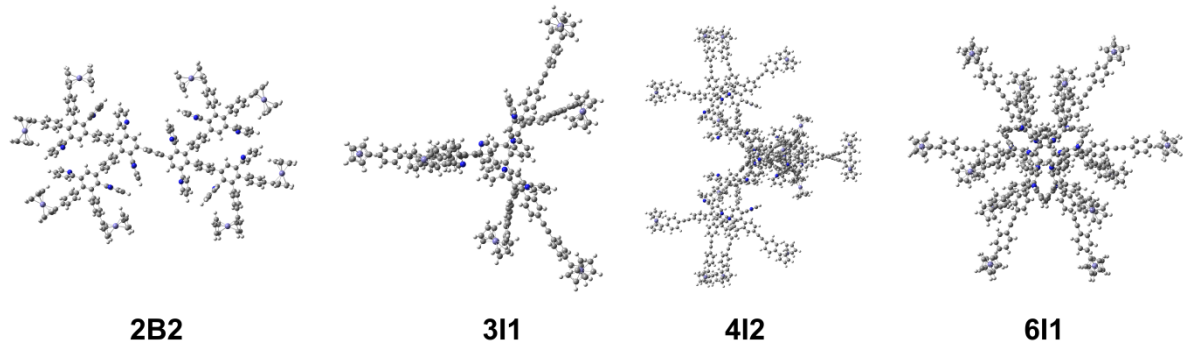


Figure 1. *Examples of dendrimers shapes.* ***nTg*** *notation:* ***n*** *– number of core branches,* ***T*** *– type of terminal groups,* ***m*** *– generation of a dendrimer.*

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1. Stewart J.J.P. "Optimization of Parameters for Semiempirical Methods VI: More Modifications to the NDDO Approximations and Re-optimization of Parameters", *J. Mol. Mod.* **2013**, *19*, 1-32. DOI: 10.1007/s00894-012-1667-x