

Characterization by SEM, TEM and Quantum-Chemical Simulations of the Spherical Carbon with Nitrogen (SCN) Active Carbon Produced by Thermal Decomposition of Poly(vinylpyridine-divinylbenzene) Copolymer

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Description of Supplementary Materials

Supplementary materials includes *.xyz files with the Cartesian coordinates of the cluster, optimized in ¹S RHF, basic units and supercell Cartesian coordinates of the models and the protocols of the computation *.out.

The name of the file consists of the system *NAME* (number of cluster – *C* or model *M*) and an addition, revealing the carbonization stage. The files like *NAMEX.** (where *X* = 0 – 12) or *NAMEY.** (where *Y* = 0 – 18) correspond to the number of the system.