COMPUTER-AIDED-DESIGN SYSTEM FOR CALCULATING ADSORPTION THERMODYNAMIC CHARACTERISTICS

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A CAD system for calculating adsorption thermodynamic characteristics has been developed which makes it possible to simulate the process of physical adsorption for molecules of various classes of organic compounds on the surface of graphitized thermal black. The system makes it possible to perform calculations for molecules capable of internal rotation, for all possible conformations. A three-dimensional model has been constructed which makes it possible to check whether the input of the molecule's initial geometric parameters is correct. It also allows exporting the data obtained to the table processor MS EXCEL for their further treatment. The system's capabilities are shown with practically important molecules as compared to experimental data.

Thermodynamic characteristics, Henri's constant, adsorption heat, adsorption, graphitized thermal black, atom-atom potentials, experiment, molecular-statistical calculation method, simulation, CAD system

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