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Enlarged Surface Meshes and Normalization Conditions for Columns and Rows of Matrices in the COSMO Method

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Earlier, normalization conditions for the columns of the PCM (Polarized Continuum Model) were determined and a method of enlarged surface meshes was developed. We developed similar methods for the COSMO (COnductor like Screening MOdel). These methods make it possible to introduce larger surface meshes without loss of accuracy and perform fast calculations of the solvation energy and the Born radii in the SGB (Surface Generalized Born) method. In addition, the corrections proposed in this work provide a significant enhancement in the accuracy of numerical calculations.

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