ELECTROSTATIC MODEL OF CRYSTAL STRUCTURE OF TETRAZINOTETRAZINTETROXIDE BENZENE SOLVATE

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Abstract: Effective charge models for isomeric molecules of tetrazinotetrazintetroxide (TTTO) of C_{2h} (I) and C_{2v} (II) symmetry as well as benzene molecule have been derived by approximation of their *ab initio* molecular electrostatic potentials with analytical potentials of point charges using FitMEP code. Energy calculations of the structure of crystalline benzene solvate II using PMC code, which involved searches for the optimal molecular packing in different spatial groups, demonstrated excellent agreement between the structure predicted as the global minimum of the potential energy surface and the experimental crystal structure.

Keywords: high-energy high-density (HEDM) compounds; method of atom–atom potentials; molecular electrostatic potential; electrostatic interaction of molecules; prediction of crystal structure; density of molecular crystals

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