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Anomalous properties of liquids for a family of models with short range tetrahedral interactions SERGEY BULDYREV, Yesiva University, GIANCARLO FRANZESE, University of Barcelona — Liquids with tetrahedral symmetry of the first coordination shell often display anomalous thermodynamic and dynamic behavior. The main reason for these anomalies is that pressurizing such liquids leads to the disordering of this local symmetry by the particles migrating from the second to the first coordination shell. This in some case may lead to the increase of entropy upon pressurizing and consequently to the volume increase upon cooling. Molecular simulations of various models with tetrahedral symmetry are able to reproduce this anomalous behavior. We study a family of simple models in which we can gradually change the degree of tetrahedrality and investigate the associated changes of the phase diagram by discrete molecular dynamics. A molecule in these models consist of a hard sphere and four point particles attached to the center of the hard sphere by directional bonds arranged in tetrahedral geometry. Each of these four particles has a narrow attractive square well so that the particles belonging to different molecules can attract to each other. We also impose a condition which does not allow a point particle in one molecule to include in its attractive well more than one point particle belonging to different molecules. We investigate how the phase diagram of the system depends on the parameters of the models. None of these models has a liquid -liquid phase transition in the accessible region of the phase. However, adding weak attractive square well to the hard sphere, or wider weak attractive square wells to the point particles can create a liquid-liquid critical point. A comparison with other simple models of the anomalous liquids is made.

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