

Poster Presentation

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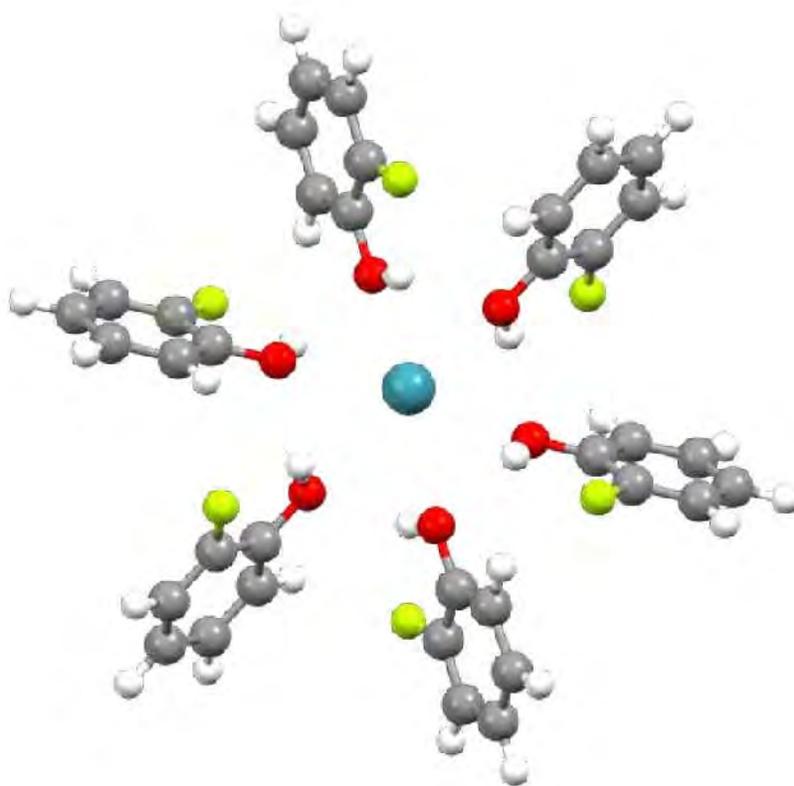
Predicting Porous Molecular Crystals and Clathrates

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The last decade has seen dramatic improvements in the theories and computer algorithms underlying computational Crystal Structure Predictions [1]. It is now possible to reliably obtain the most likely crystal structures of at least simple molecules starting from nothing more than a drawing of the molecule. We can now go even further and look for rare and exotic kinds of crystals such as porous molecular crystals, clathrates and inclusion compounds among our predictions and calculate their physical properties [2], paving the way for the “science of hypothetical materials”. In our poster, we present results on the prediction of fluorophenol xenon clathrates. We have performed crystal structure predictions by global lattice energy searches on o- and m-fluorophenol. The predicted structures have then been analyzed for porosity and their likelihood of being clathrates. From the several thousands of predicted structures, we select a few likely candidates according to an empirical rule based on the guest to host volume ratio [3]. Results from solid state xenon-129 NMR indicate that we have successfully determined the crystal structures of both o- and m-fluorophenol xenon clathrates and we suggest that Crystal Structure Prediction in combination with xenon-129 NMR is a powerful method for determining the structures of clathrates in general.

[1] G. M. Day, T. G. Cooper, A. Cruz-Cabeza, et al. *Acta Cryst*, 2009, B65, 107-125, [2] A. Cruz-Cabeza, G. M. Day, W. Jones, *Chemistry - A European Journal*, 2009, 15, 13033–13040, [3] K. Nakano, K. Sada, Y. Kurozumi, M. Miyata, *Chemistry - A European Journal*, 2001, 7, 209–220



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