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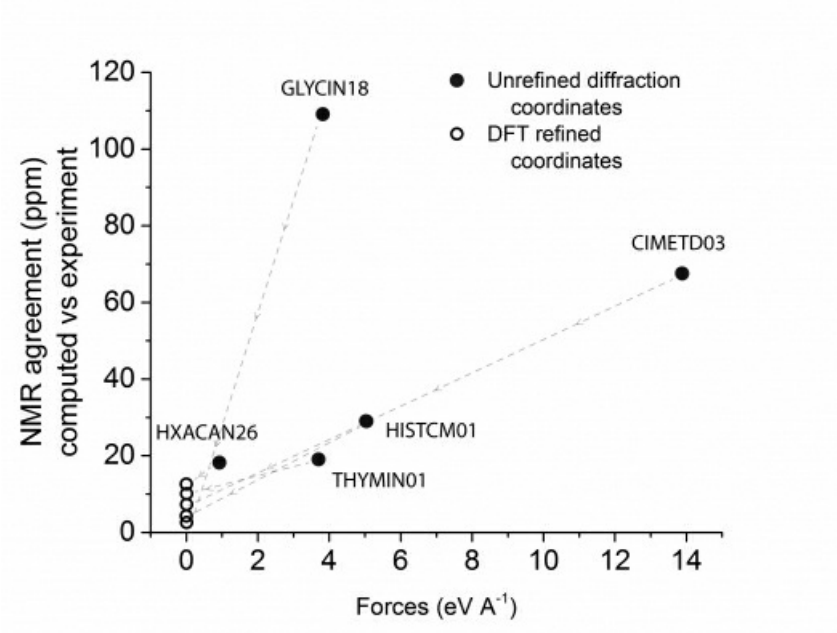
Predicting and refining crystal structures with NMR data

James Harper[1]
[1]*Department Of Chemistry, University Of Central Florida, Orlando, United States*
E-mail: James.Harper@ucf.edu

Theoretical crystal structure predictions (CSP) usually ranks candidates by lattice energy. Despite significant recent progress, the consistent selection of a correct structure remains challenging and is largely limited to rigid structures. This presentation explores an alternative in which NMR parameters are calculated for candidate structures then compared with experimental data to obtain rankings. This approach is demonstrated to eliminate approximately 90% of CSP candidates when carbon-13 data are employed and lattice effects are ignored.[1] Inclusion of lattice fields significantly improves selectivity and allows a single correct structure to be consistently chosen.[2] An important component of these studies is the discovery that an ab initio refinement of geometry is required in to ensure accurately selection.[2] Surprisingly, most published crystal structures can also be improved by a lattice-including refinement.[3] Several NMR parameters are able to track and guide these refinements, but they are largely undetectable by conventional diffraction methods. This "NMR crystallography" approach to refining and improving certain crystal structures is illustrated using lauric acid and other small organic structures.

[1] Harper, J. K. and Grant, D. M. (2006). Cryst. Growth Des., 6, 2315–2321.
[2] Kalakewich, K. et al.(2013) Cryst. Growth Des. 13, 5391–5396.
[3] Harper, J. K. et al. (2013) CrystEngComm, 15, 8693–8704.



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