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ShiftML. A machine-learning model for chemical shifts in molecular crystals with uncertainty quantification

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NMR cristallography is gaining traction as a tool to achieve structure determination for molecular materials, but it relies on computationally-demanding electronic structure calculations to estimate the chemical shieldings of candidate structures.
Here I discuss the construction of a machine-learning model trained on electronic-structure data, that can predict accurately chemical shieldings in molecular materials containing C, H, N, O, S, and that incorporates an uncertainty estimation model that makes it possible to assess quantitatively its reliability for different compounds.
I will demonstrate that it can substitute for electronic-structure calculations to support NMR crystallography, and discuss how it can be combined with a Bayesian framework to determine the confidence of NMR-based structural determination.

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