

## MS36 Software development in quantum mechanics-based methods of crystallography

MS36-02

Neural network predictors in quantum chemical topology

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### Abstract

Quantum Chemical Topology (QCT) [1] has played a prominent role in the interpretation of high accuracy XRD experiments and in the development of Quantum Crystallography [2]. Basic to this framework are atomic charges, which need from expensive 3D numerical integrations. QCT charges are particularly attractive given their invariance against orbital transformations. Given that Machine Learning (ML) techniques have been shown to accelerate orders of magnitude the computation of a number of quantum mechanical observables, we take advantage of ML knowledge to develop NNAIMQ [3], an intuitive and fast Neural Network (NN) model for the computation of QTAIM charges for C, H, O and N atoms with high accuracy. Our model has been trained and tested using data from quantum chemical calculations in more than 45 000 molecular environments of the near-equilibrium CHON chemical space. The reliability and performance of NNAIMQ have been analyzed in a variety of scenarios. Altogether, NNAIMQ yields remarkably small prediction errors, well below the 0.03 electron limit in the general case, while accelerating the calculation of QTAIM charges by several orders of magnitude. Generalization to other descriptors is also proposed.

### References

- [1] R. Bader, *Atoms in Molecules: A Quantum Theory*, International series of monographs on chemistry (Clarendon Press, Oxford, 1990), ISBN 9780198551683
- [2] S. Grabowsky, A. Genoni, H. Bürgi, *Hans-Beat Chemical Science*. 8, 4159–4176, 2017.
- [3] M. Gallegos, J. M. Guevara-Vela, A. Martín Pendás, *J. Chem. Phys.* 156 014112, 2022