PARTITION FUNCTION ESTIMATION FROM INCOMPLETE SPECTROSCOPIC GRAPHS

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Statistical mechanical treatment of molecules is a crucial part of the analysis workflow for many fields, ranging from reaction dynamics, spectral intensity simulation, to abundance characterization in the interstellar medium, to materials research and simulation. At the heart of this is computation of the partition function—the statistical equivalent to the quantum mechanical wavefunction—which involves summation over thermally relevant energy levels. Despite being conceptually straightforward, calculation of the partition function can be a challenging task: at high temperatures, the number of contributing states grows exponentially, and often the list of states is truncated for computational and portability reasons.

Here, we propose the use of physics informed graph neural networks to parameterize the partition function calculation based off incomplete spectroscopic graphs, and as a proof-of-concept, demonstrate its applicability and weaknesses through the study of pure rotational energy levels. In contrast to approximate analytical expressions based on the principal rotational constants, graph structures natively capture effects such as centrifugal distortion of varying degrees, which otherwise significantly undermine the accuracy of calculated partition functions at elevated temperatures. As part of our study, we discuss implications on computational performance, data requirements, and applicability in typical workflows.