

Abstract

In Putz M.V. (ed.), *Quantum Frontiers of Atoms and Molecules*, Nova Science Publishers, Inc., New York, NY, USA, p. 479-497 (2011) ISBN 978-1-61668-158-6.

Dehmer M., Emmert-Streib F., Tsoy Y.R., Varmuza K.:

Quantifying structural complexity of graphs: Information measures in mathematical chemistry

In this chapter, we give a conceptional view about information measures for graphs which can be used to quantify their structural complexity.

We focus on treating such measures in the context of mathematical chemistry but we want to mention that those are also applicable for arbitrary complex networks. Besides reviewing the most known information indices often used in chemical graph theory, we propose an information functional that is based on degree-degree associations in a graph. This leads us to a parametric graph entropy measure to quantify the structural information content of a graph. A brief numerical example shows how the measure can be calculated explicitly.