Review on PhD thesis of Mgr. Jiřího Hostaše:
Accurate Quantum Mechanical Calculations on Noncovalent Interactions: Rationalization of X-ray Crystal Geometries by Quantum Chemistry Tools.

The thesis deals with extended studies of non-covalent interactions using ab initio, and DFT calculations.

The topics of study are shortly presented in part Introduction. Here, basic data and approximations are very shortly mentioned. Necessary computational tools are described clearly (which I highly appreciate) and practically without serious mistakes in part Methods. All the results are briefly but sufficiently addressed in part Projects where all main goals of the thesis are described and documented also using 27 Figures and 11 Tables.

The submitted thesis clearly demonstrates huge amount of work, which was successfully published in prestigious journals like J.Chem.Theory&Comp., J Am. Chem. Soc. or Chem. Eur.J.
Mgr. Hostaš is the first author in four of these papers. More over another two papers were produced within his PhD studies in the group of Prof. Hobza.

I would also like to stress broad scope of the interests of Mgr. Hostaš going from general semiempirical methods to highly correlated ones applied on simple molecules as well as on large biomolecular systems.

Finally I would like to conclude that the thesis proves the author's disposition to creative and independent scientific work and I recommend awarding Mgr. Jiří Hostaš with the scientific degree „Philosophiae doctor".

In Prague, April, 10 2017

Prof. Jaroslav Burda, DrSc.