Report by Carlo Gatti on the PhD thesis of Francesco F. Summa on Molecular Properties via Induced Current Densities

General judgement: The PhD thesis written by Francesco F. Summa on *Molecular Properties via Induced Current Densities* is a careful report of a highly qualified and innovative research. Sixteen peer-reviewed publications on renowned journals in the chemical physics and theoretical chemistry areas have originated from the work reported in the thesis, besides other six publications, also co-authored by F. F. Summa on different subjects. The number, excellent quality and originality of the 16 papers mentioned above is far beyond any usual standard for a PhD student, even when the worldwide reckoned scientific excellence of the research group(s) within which the work has been performed is properly taken into account.

The work done in the thesis consists of three well identified parts: theory development, SW implementation of the developed theory into the freely available SYSMOIC package and test applications of the newly developed theory and SW on a good number of carefully selected cases.

All three mentioned steps of the PhD work are reported in the thesis with great clarity, perfect progression and concatenation. The writing is terse and quite accurate. After a brief and clear introduction, the general quantum mechanical framework for the treatment of a molecular system interacting with electric and magnetic time dependent fields is elegantly recapped and exposed. Chapter 3 introduces the equations defining the total current density induced by a time-independent magnetic field and illustrates in detail the procedures aimed at solving the problem of the origin dependence of the computed current density vector field. Chapter 4 deals with time-dependent perturbations and how they do result into time-dependent charge and current densities. Chapter 5 reports a number of very interesting applications, both in the static and in the dynamic regimes, of the theoretical and SW developments illustrated in the Chapter 3 and 4. The work performed in the thesis and the writing thereof both show a very high command of symmetry analysis of systems in a magnetic field and of the topological analysis and classification of current densities, two subjects which are not at all trivial. The provided list of acronyms, in the initial pages of the thesis, is highly appreciated. Overall, this thesis provides an extremely recommendable reading for those who are interested or want to be acquainted with the most recent progresses on the subject of *Molecular Properties via Induced Current Densities*

Based on all what said above, the thesis of Francesco Summa can be presented at the oral PhD exam as it is. The suggested revisions (see below) are to be considered as recommended but not cogent.

These are the two points that I suggest to consider in what would represent a very minor revision of the thesis:

a) Section 5.4 on the H-Bonds Characterization in Cyclododecapeptoids should be probably removed. It has no relation with the other parts, it has no apparent scope (at least this is not declared) and at the present stage this section represents more an exercise rather than a true piece of research. Surely, Section 5.4 it is not at the same top level of the preceding sections.
b) Section 5.4 could be replaced by giving some more detail on the very interesting studies of electron correlation effects on the induced current densities (namely, that part of the thesis work performed during the stay abroad of the candidate, whose preliminary results are reported in poster 3)

Carlo Gatti (former Dirigente di ricerca, presently retired, at CNR-SCITEC, Milano)

Milano, 21/12/2022