

TopChem *Web* - a free web interface for Quantum Chemical Topology

<http://topchemweb.sorbonne-universite.fr/>

TopChem*Web*
LCT SORBONNE UNIVERSITE CNRS

What is TopChemWeb ?

TopChemWeb is a web-based implementation of the TopChem2_code which is a stand-alone program for advanced and robust topological analyses of the electron density (RHO), the electron location function (ELF), and non-covalent interactions (NCI).

Topchem2 calculations submitted: if all goes well, you will receive an email with a link to the TopChemWeb Results website. There you will find a graphical interface to view your results as well as the possibility to download all results files.

Limitations: on the wfn/wfx file specifications.

Submit TopChem2 job

wfn/wfx file: input current Gaussian wfn/wfx file. Limits : 5Mb, 12 atoms, 400 primitives.
function: compute the three-dimensional grid and enable the basin analysis.
Search critical points: yes (enabled) / no (disabled) / only (enables only the search of critical). The default is no.
refine: yes (enabled) / full (all points are assigned). Additional refinement step at the final stage of the basin analysis. Default: y
proc: number of used processors for the basin analysis. Default: 1



Your Name

required fields

Academic email address

Upload your structure (WFN/WFX format)

atoms primitives

Calculation options

Function
 rho elf nci

Search critical points
 no yes only

Refine
 yes full

Number of Processors

© 2023 Laboratoire de Chimie Théorique, Sorbonne Université.
Last modified: August 21 2023.

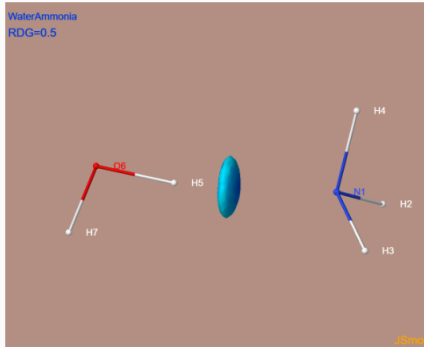
Graphical interface for viewing results (rho, ELF or NCI)

TopChem*Web*
LCT SORBONNE UNIVERSITE CNRS

Results

job id: 64e30774b211e
date: 21-8-2023
function: NCI

10.77 MB



WaterAmmonia
RDG=0.5

isosurfaces: opaque | translucent | mesh

© 2023 Laboratoire de Chimie Théorique, Sorbonne Université.
Last modified: August 21 2023.

