

High Performance Computing (HPC) Cluster

High performance computing cluster:

High-performance computing cluster can be utilized to perform electronic structure calculations of molecules which are of interest to chemists. Various commercial as well as freeware are already installed in the cluster for calculations.

Make and Model:

45 node Fujitsu HPC cluster

Specification/ Features:

- 45 nodes (2x12 core intel) processors with 4GB per core RAM and 25TB Parallel file system

Available mode of use:

- Gaussian-09
- MOLCAS
- ORCA
- GROMACS

Whether the facility is open to external users: Yes
(Only for Chemistry department groups)

Location:

Room no: HPC data centre, Computer room (II Floor)

Department: Department of Chemistry

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