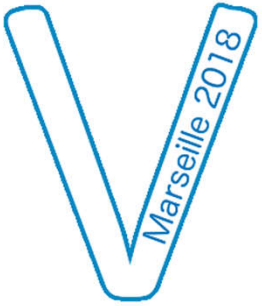

VALBO

Understanding Chemistry and Biochemistry with Conceptual Models

Glance at XMVB
Program and Exercises

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Platforms and Compilers

- *NIX platforms:
  - Linux
  - Mac OS X
  - AIX
- Windows (with CMD)
- Compilers supported:
  - GNU
  - INTEL suite
  - PGI
  - XLF on AIX

Tools in XMVB

- Prepare integrals: preint
- XMVB program: xmvb
- Orbital Visualization: moldendat.exe
- Cartesian to spherical: 6d25d.exe
- NBO guess: nboprep.exe

Methods and Algorithms

- VBSCF
  - Numerical/Analytical gradients
  - Full Hessian
  - RDM-based VBSCF
  - Tensor-based VBSCF
- BOVB
- VBCI(S/SD/DS)
- icVBPT2
- DFVB
- Solvation models
  - VBPCM
  - VBEFP

CD and Parallelization

- Cholesky Decomposition for ERIs
  - Reduce the memory consumption
  - Accelerate the construction of Fock and Hamiltonian matrices
  - Available for RDM-/tensor-based VBSCF
- Parallelization: OpenMP
  - Available for all methods
  - No need for MPI
  - OMP_NUM_THREADS for NCPU

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Logging in and Run XMVB

- Logging in with SSH, i.e.

  ssh vb@172.16.56.26

  and type the password
- Run XMVB
  - Computer with 32 cores and 256GB memory
  - XMVB is proceeded with a batch script ***subxmvb xmi***
  - 4 processors will be used for an XMVB job

Procedure of Calculations

- General procedure of an XMVB calculation
  - Integral and initial guess preparation
  - XMVB input preparation
  - Run XMVB
- To proceed BOVB
  - Run VBSCF calculation first
  - Run BOVB with VBSCF orbitals
- To proceed VBCI
  - Run VBSCF with “BOYS”
  - Run VBCI with VBSCF orbitals

Exercises: Brief Overview

- Directory “answers” in every exercise
  - To check your results
  - Try to finish the exercises without the answers
- 4 paper exercises: “basis” of VB theory and XMVB calculations
- 10 computer exercises to learn how to proceed XMVB calculations and get information from the results

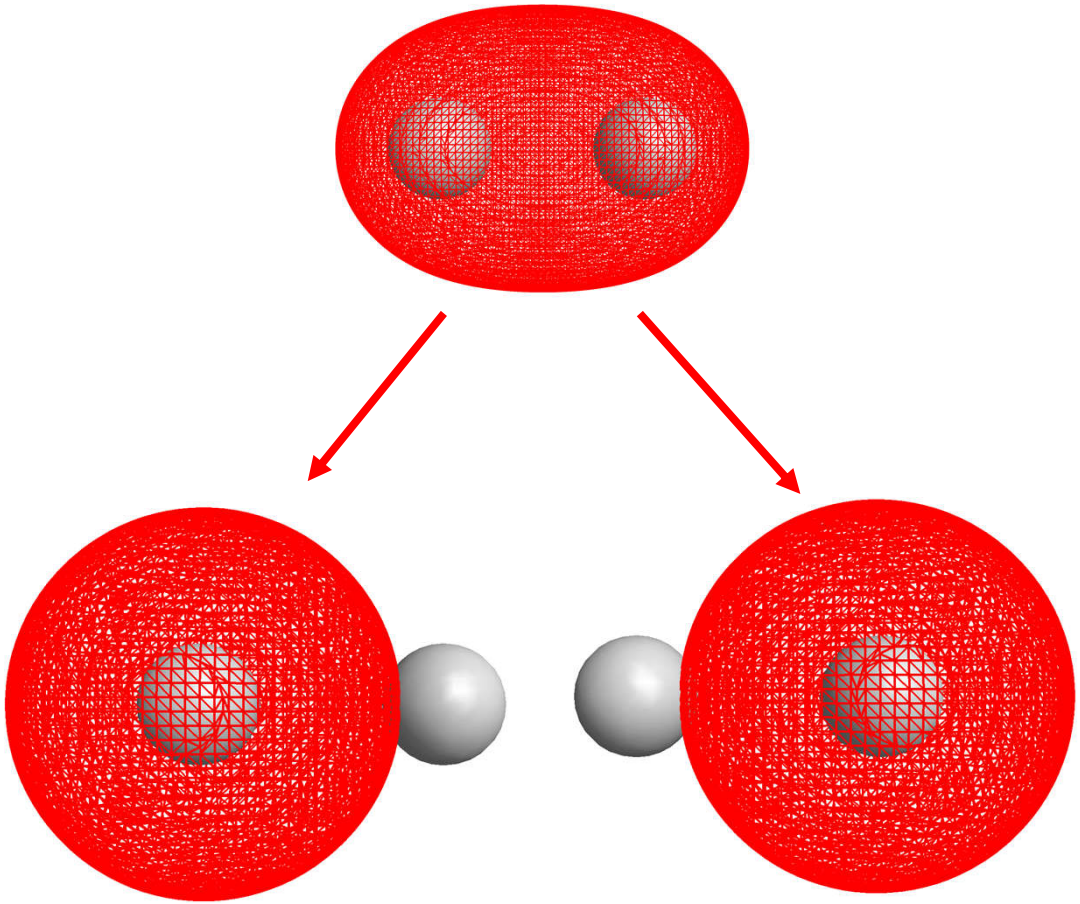
Computer Exercises

- Start from HF molecule
  - Input files are prepared in this exercise
  - To know the procedure of VBSCF calculation
  - To understand the keywords/sections
  - To get information from the output
- Prepare (part of) your input files in the other exercises, or fix errors
- Compute properties such as REs, BDEs, $E^{\neq}$, etc. in different levels
- Try different initial guesses
- Compare similar bonds and find difference.
- Understand the physics/chemistry behind the numbers.

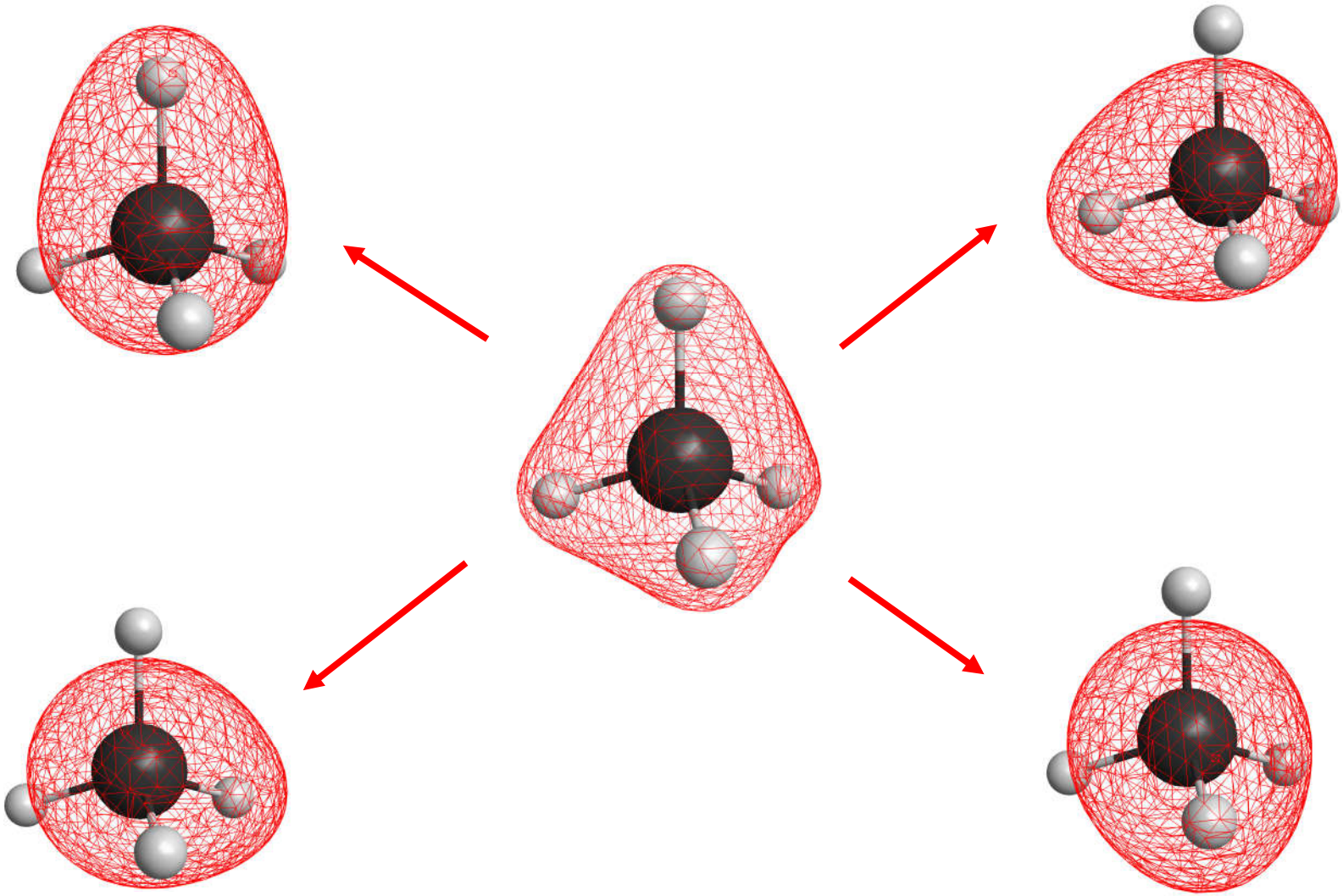
Key Points

- How many sections are there in an input file? What do they mean?
- What's resonance energy? How to calculate?
- How do the weights change as the correlation energy is involved?
- For π systems such as O_3, SO_2, benzene and anthracene, how to deal with the inactive σ orbitals? Why?
- How shall we pick up essential structures?

Initial Guess From MOs: H_2



Initial Guess From MOs: CH_4



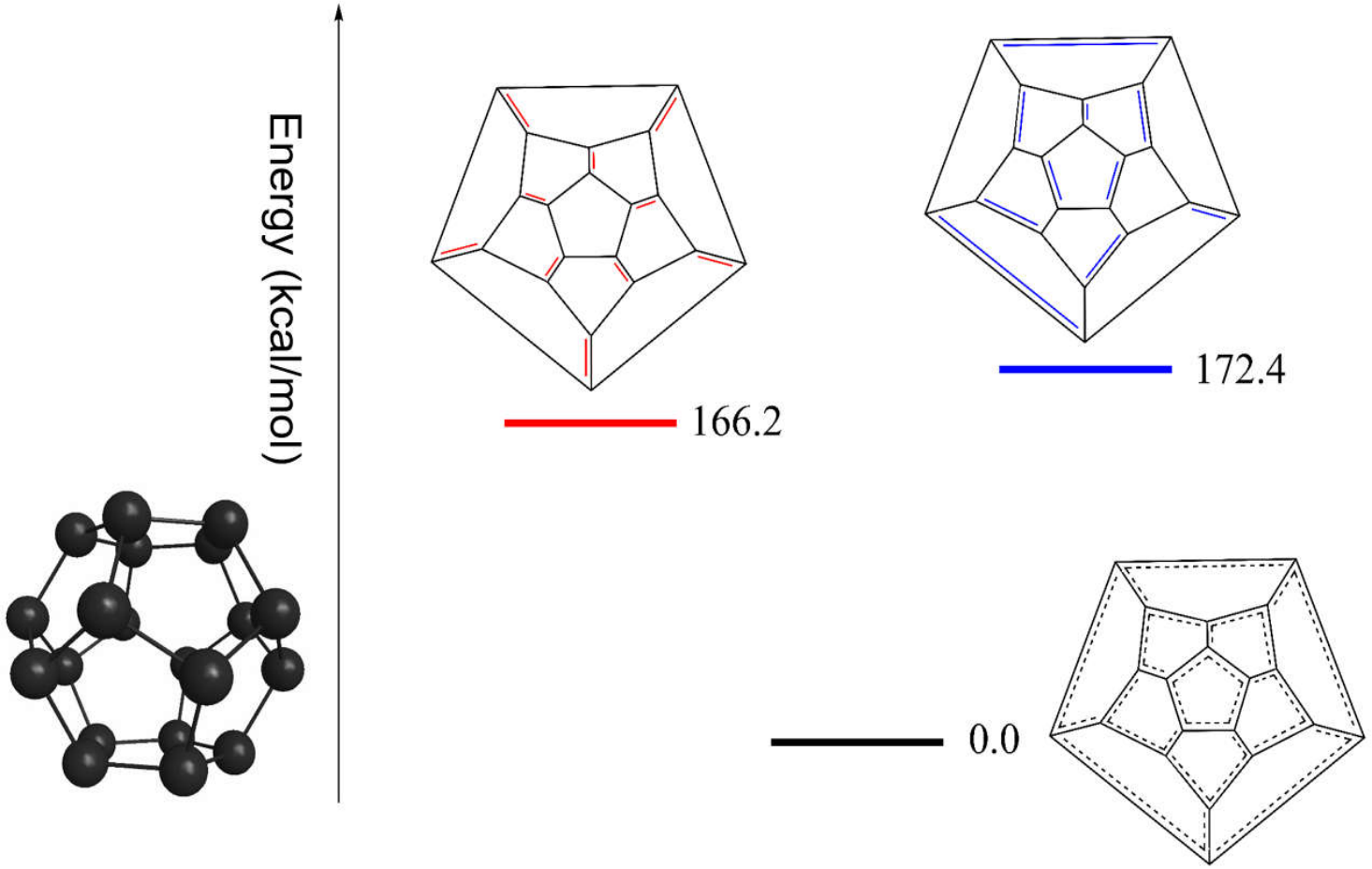
Try you best

Thank You for Your Attention!

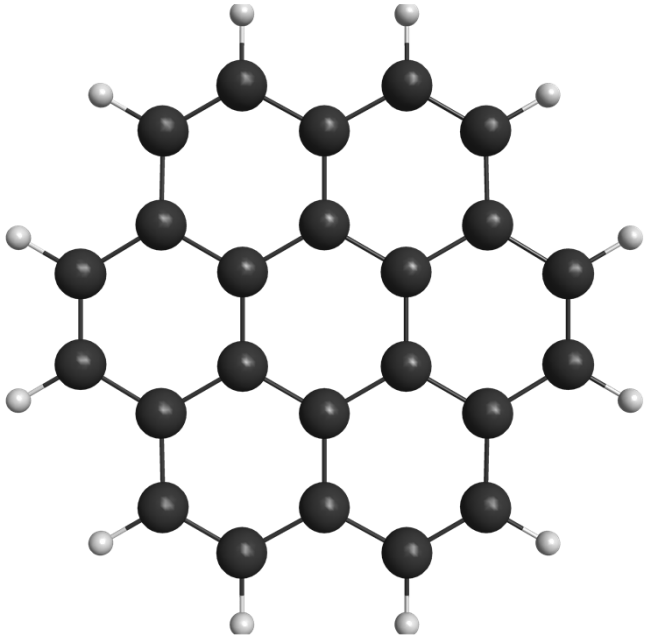
Limit of system size

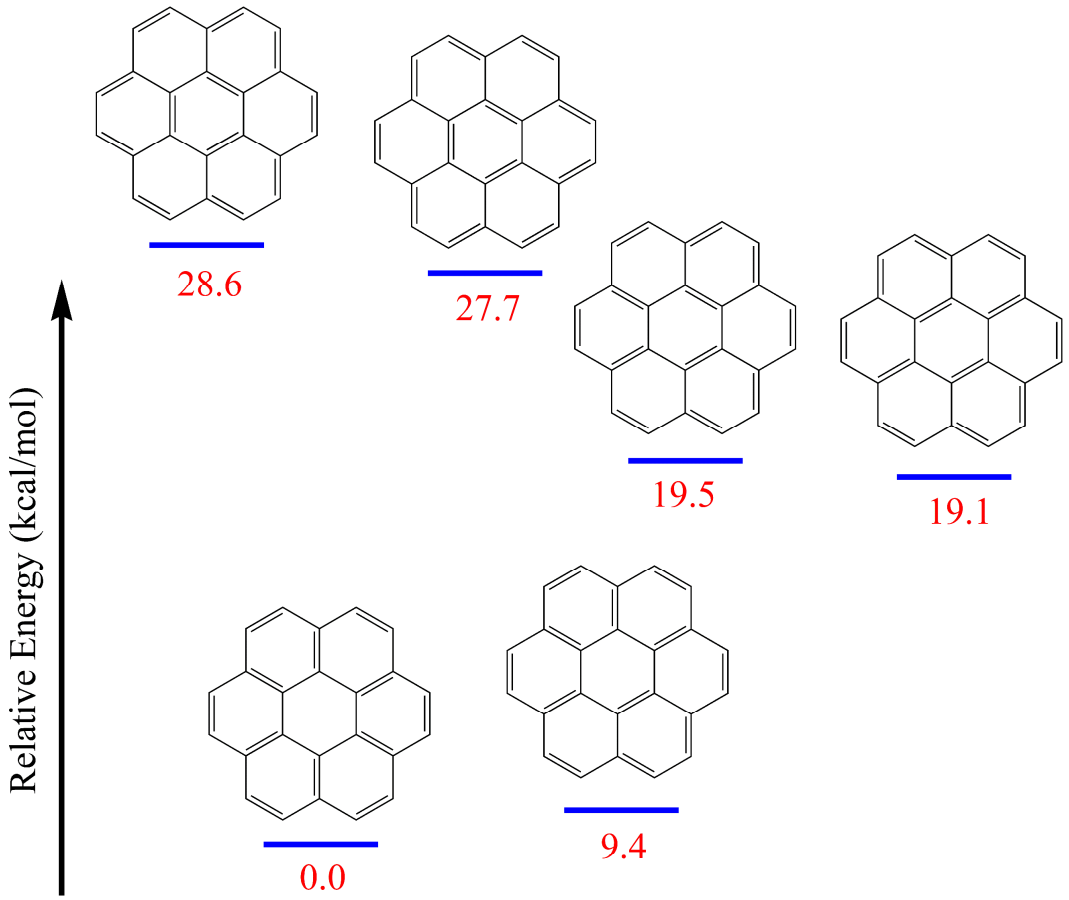
- 1000 basis functions (with CD)
- Size of active space (tensor-based):
  - (18,18) for all structures
  - (22,22) for covalent structures
  - (24,24) for a few structures (i.e. Kekulé only)

Limit of system size



Limit of system size





Basis set: 6-31G*