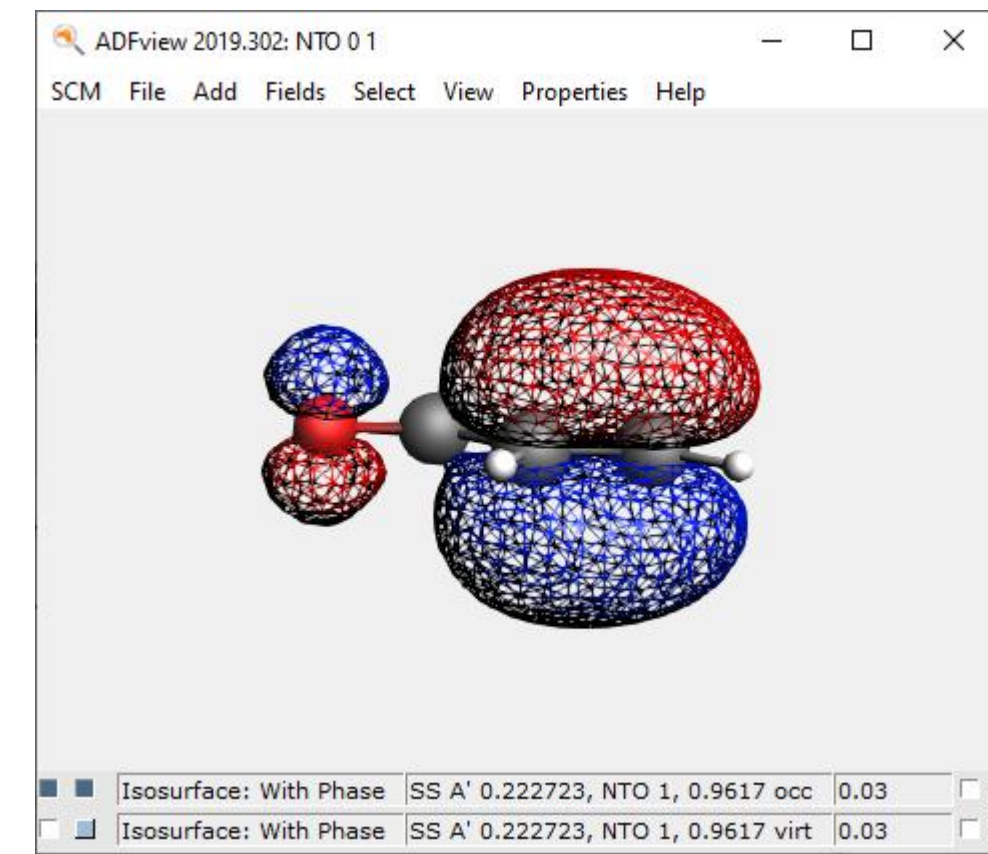
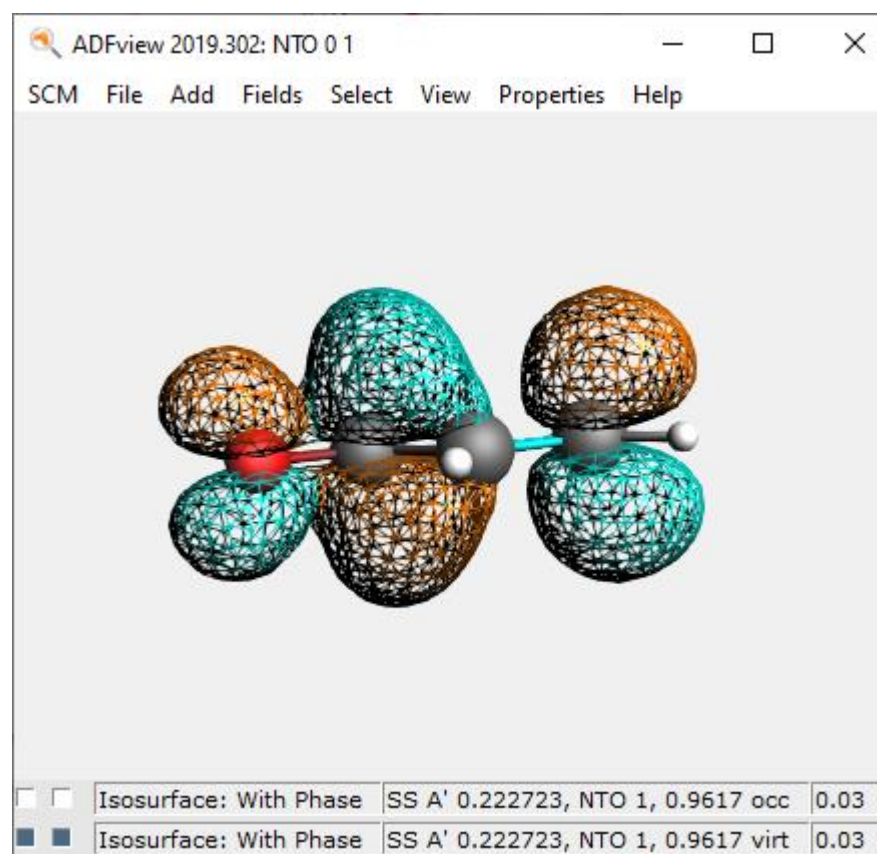
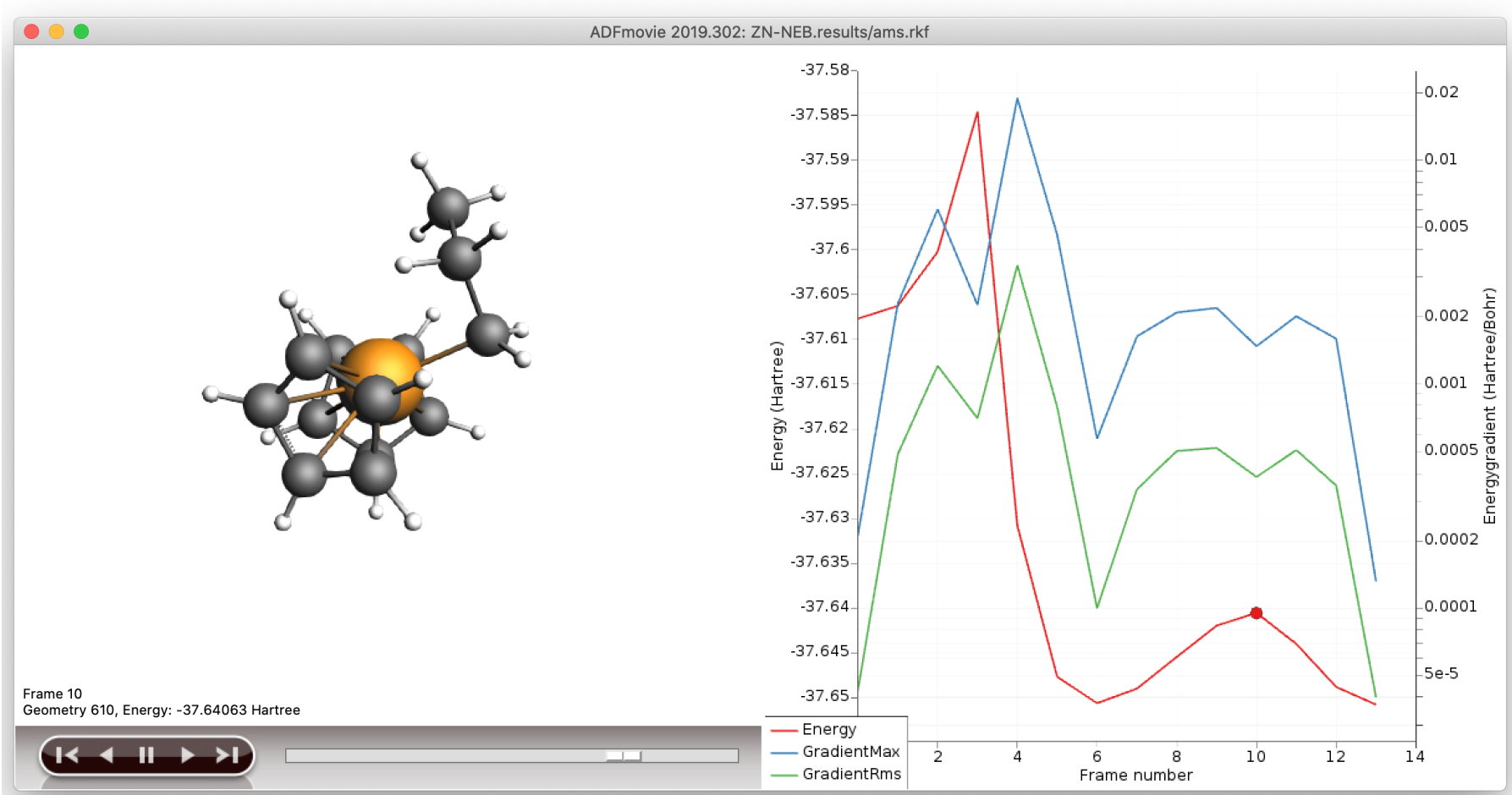
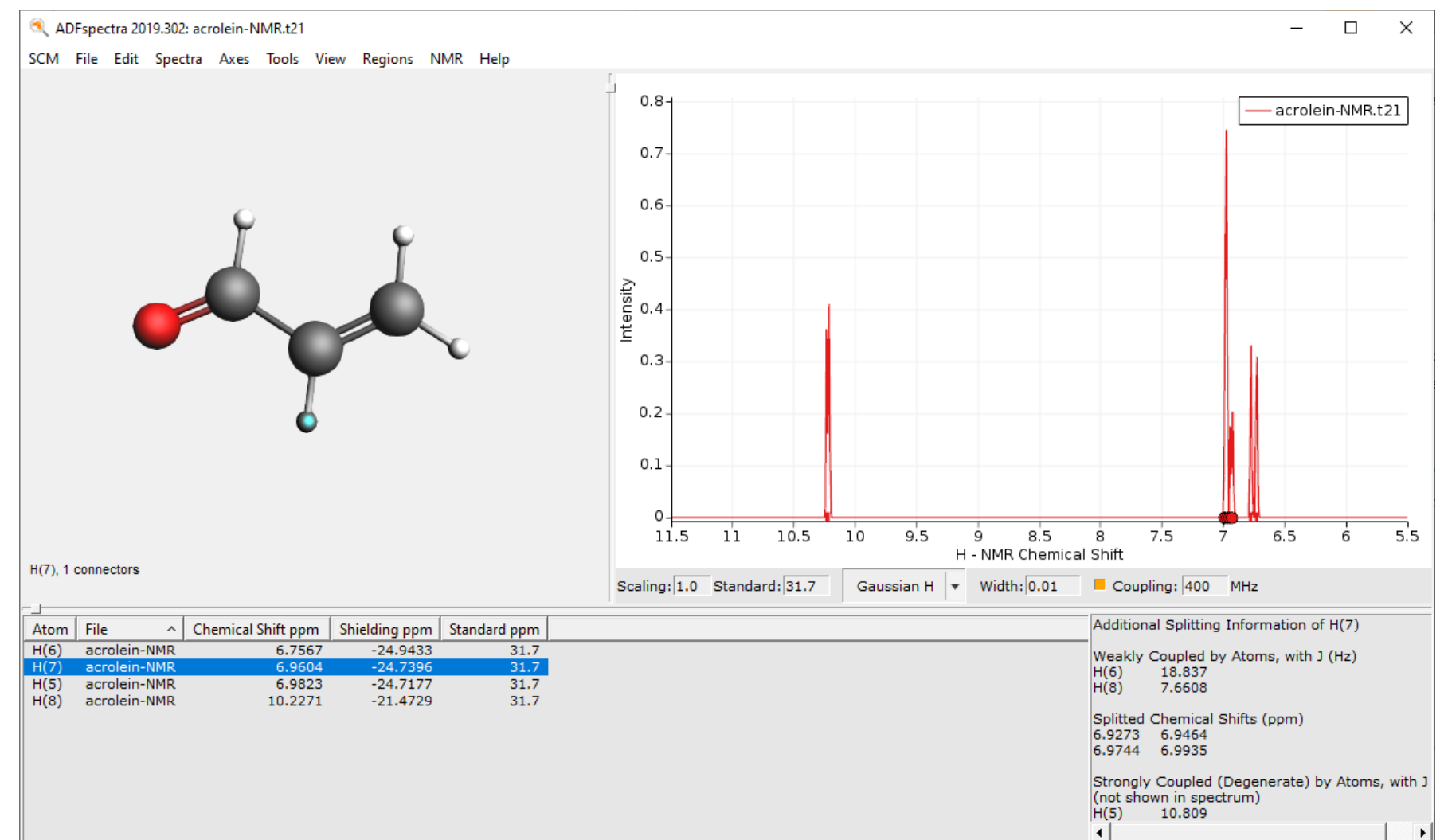
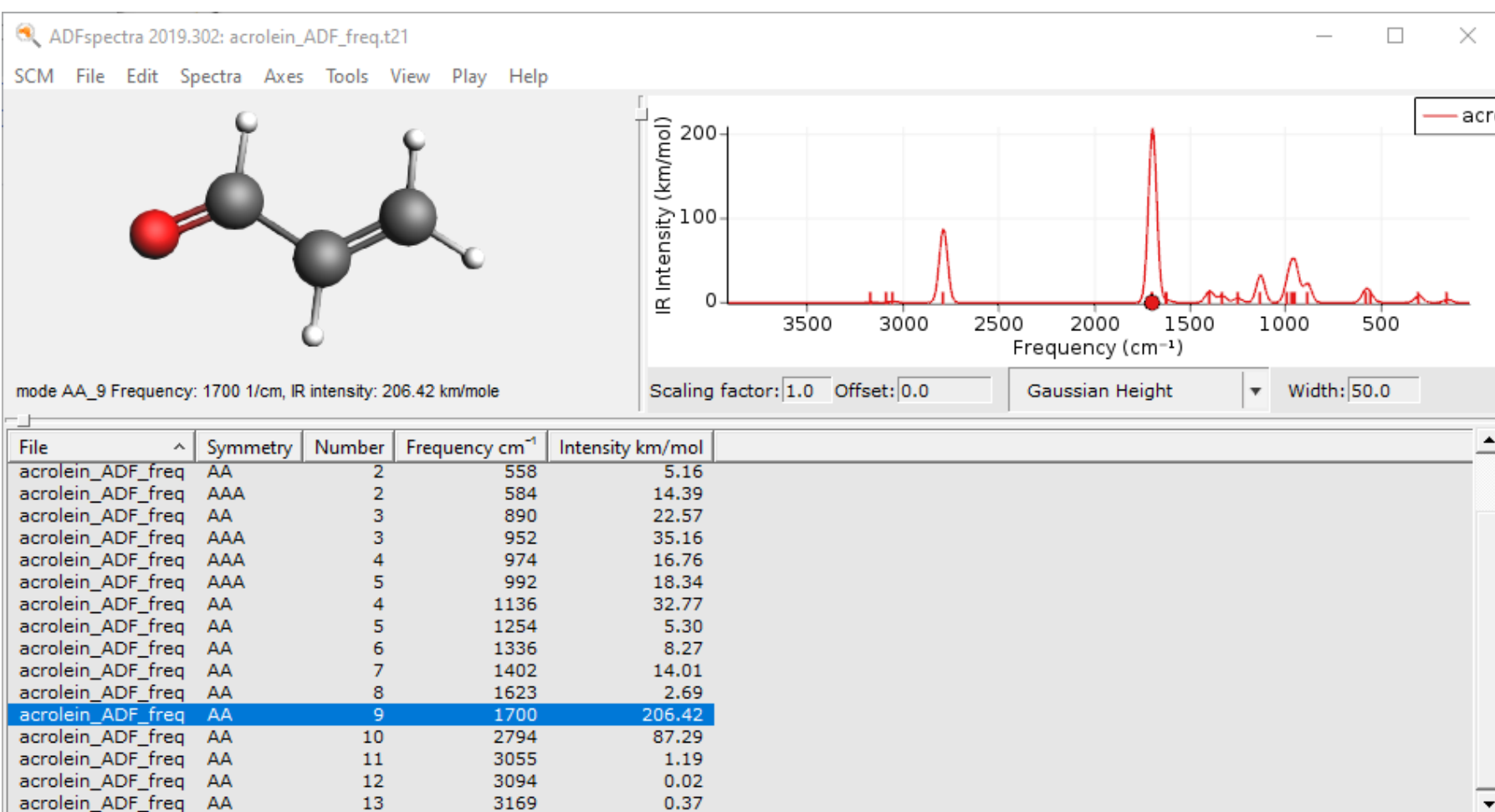


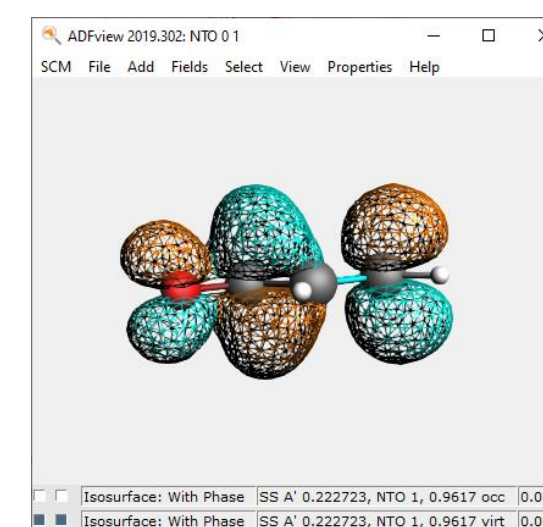
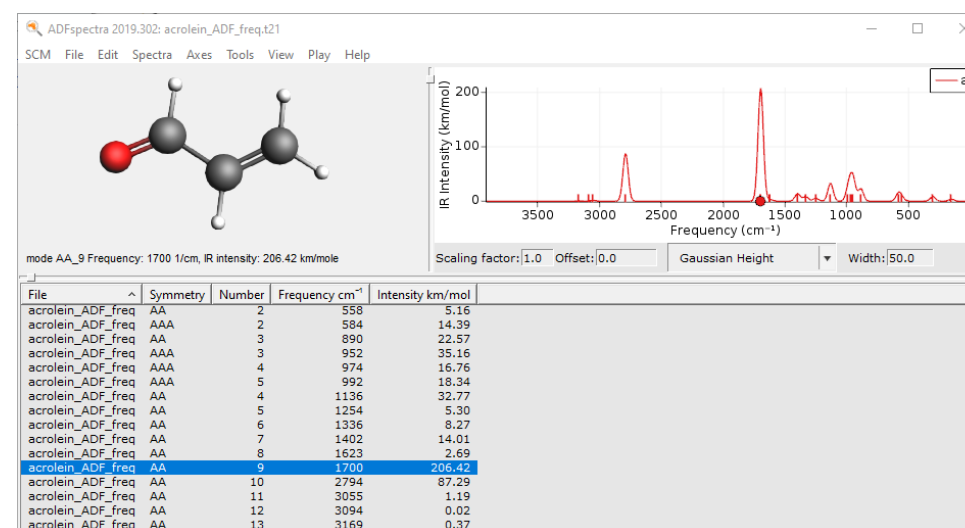
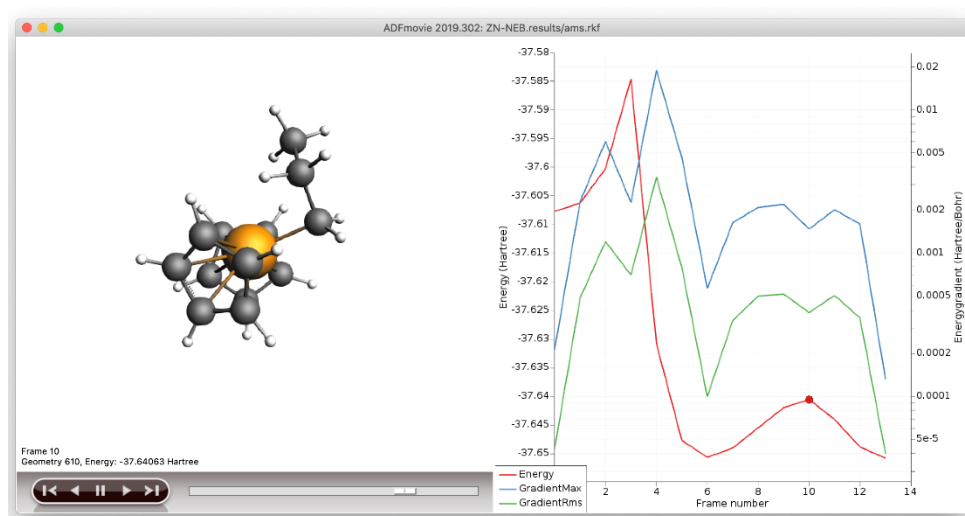
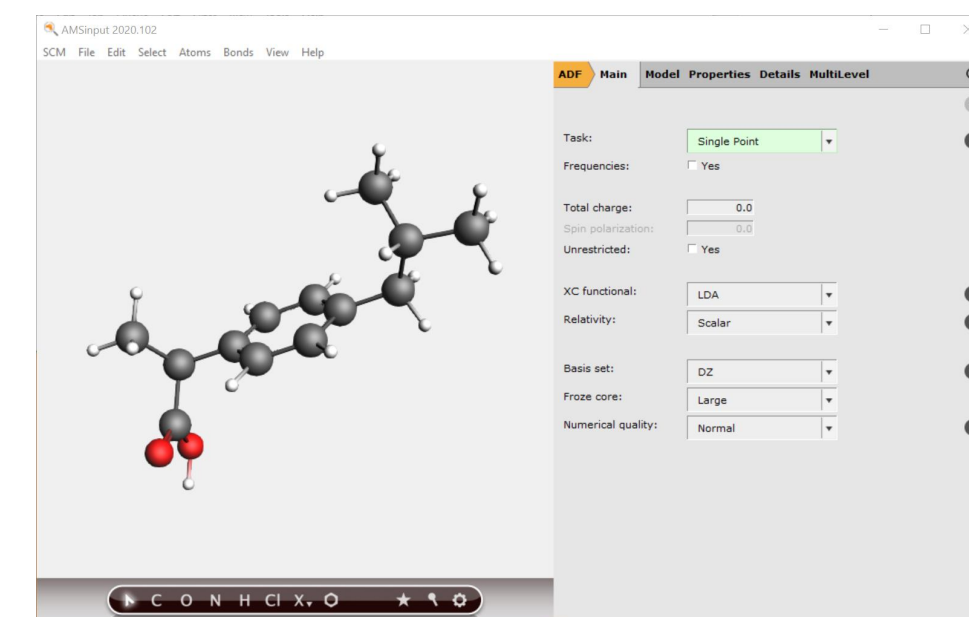
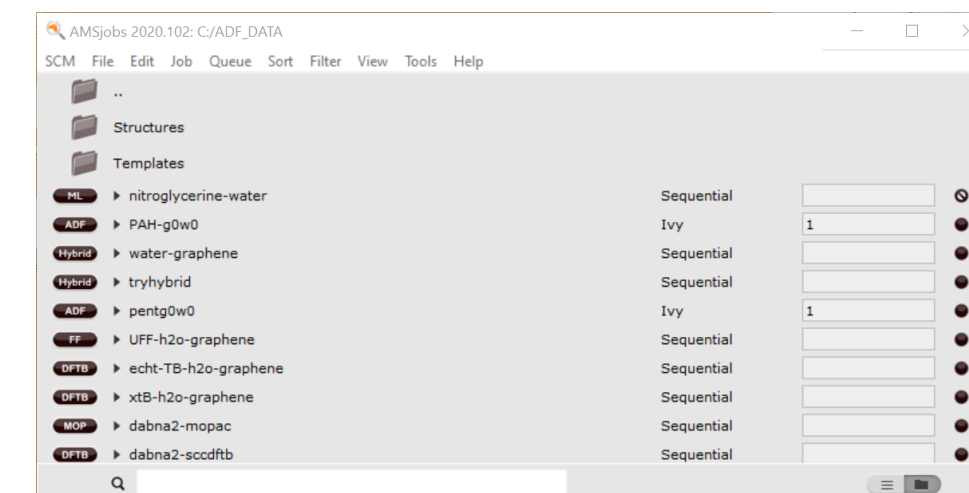
# Getting started with AMS!



# Getting started with the GUI

## Starting AMSjobs: job bookkeeping

- Win: dbl-click desktop item
- Mac: open Application
- Linux: run `$AMSBIN/adfjobs`
- AMSInput: define system + properties + settings
- Other: (View, Levels, Movie, Spectra, Band Structure, AMSTrain, Microkinetics, COSMO-RS, KF Browser...)
  - Open from result file, SCM menu or e.g. by dbl-clicking 'amsinput.exe' (Win) or running '\$AMSBIN/amsinput'



# AMSjobs: job bookkeeping

switch GUI module

define & switch queues  
([remote queues](#))

reports & templates

job status

see files for this job

change default, e.g.  
cores, nodes, walltime

queue

The screenshot shows the AMSjobs GUI window titled 'AMSjobs 2020.102: C:/ADF\_DATA'. The menu bar includes SCM, File, Edit, Job, Queue, Sort, Filter, View, Tools, and Help. The left sidebar shows a file tree with folders for 'Structures' and 'Templates', and a list of jobs with their types (ML, ADF, Hybrid, FF, DFTB, MOP) and names. The main area displays a table of jobs with columns for 'queue' (Sequential, Ivy) and 'status' (represented by icons). A search bar is at the bottom left, and a toggle for 'all jobs / folder view' is at the bottom right.

Job Type	Job Name	Queue	Status
ML	nitroglycerine-water	Sequential	⊘
ADF	PAH-g0w0	Ivy	●
Hybrid	water-graphene	Sequential	●
Hybrid	tryhybrid	Sequential	●
ADF	pentg0w0	Ivy	●
FF	UFF-h2o-graphene	Sequential	●
DFTB	echt-TB-h2o-graphene	Sequential	●
DFTB	xtB-h2o-graphene	Sequential	●
MOP	dabna2-mopac	Sequential	●
DFTB	dabna2-sccdftb	Sequential	●

job type

search

all jobs / folder view



# Basic calculations & settings

The screenshot shows the AMSinput 2020.102 GUI. The main window displays a molecular structure on the left and a settings panel on the right. The settings panel is divided into tabs: ADF, Main, Model, Properties, Details, and MultiLevel. The ADF tab is selected, showing various calculation parameters. Annotations in yellow boxes point to specific features:

- switch engine**: Points to the ADF tab.
- job types & set up**: Points to the Main tab.
- search**: Points to the search icon in the top right corner.
- job type**: Points to the Task dropdown menu, which is set to Single Point.
- charge/spin**: Points to the Total charge and Spin polarization input fields, both set to 0.0.
- functional & relativistic appr**: Points to the XC functional dropdown menu, which is set to LDA.
- basis & numerical accuracy**: Points to the Basis set dropdown menu, which is set to DZ.
- builder tools**: Points to the molecular structure editor at the bottom left.
- preoptimize**: Points to the preoptimize button at the bottom center.
- symmetrize**: Points to the symmetrize button at the bottom center.
- > = more details**: Points to the right arrow icon in the settings panel.

The molecular structure editor at the bottom left shows a molecule with atoms represented by spheres (C, O, N, H, Cl, X) and bonds. The settings panel on the right includes the following parameters:

- Task: Single Point
- Frequencies: ☐ Yes
- Total charge: 0.0
- Spin polarization: 0.0
- Unrestricted: ☐ Yes
- XC functional: LDA
- Relativity: Scalar
- Basis set: DZ
- Froze core: Large
- Numerical quality: Normal

SCM logo is visible in the bottom left corner.

# GUI input editor controls

- ▶ Free rotation **left mouse button (LMB)** & drag
- ▶ In-plane rotation **ctrl + LMB** & drag
- ▶ In-plane shift **right mouse button (RMB)** & drag
- ▶ Zoom **mouse wheel / alt** & drag
- ▶ Area selection **shift + LMB**
- ▶ Deselect **LMB** on drawing space
- ▶ Undo **ctrl + Z**
- ▶ Redo **shift + ctrl + Z**
- ▶ View along x- / y- / z-axis **ctrl + 1 / ctrl + 2 / ctrl + 3**

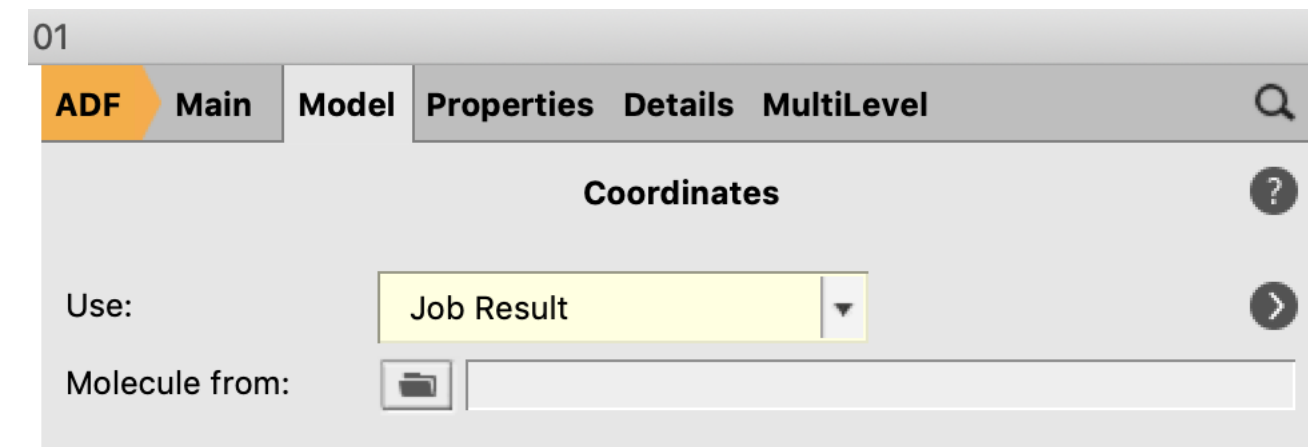
# GUI input editor controls

- ▶ Selection free rotation **LMB** & drag from a selected atom
- ▶ Selection in-plane rotation **ctrl** + **LMB** & drag from atom
- ▶ Selection in-plane shift (**shift** +) **RMB** & drag from atom
- ▶ Select all atoms **ctrl** + **A**
- ▶ Add hydrogen atoms **ctrl** + **E**
- ▶ Link selected atoms **ctrl** + **L**
- ▶ Delete selected atoms **del** / **backspace**
  
- ▶ More shortcuts: **Help** → **Shortcuts**

# Using the GUI more efficiently

## 1. Chained jobs

- Model -> coordinates use Job results
- E.g. first do pre / partial optimization
- Can not be used to also read in Hessian
  - Python scripting could work (do check on nimag e.g.)



## 2. Preset

- If you always use same XC, basis set, relativity & quality, etc. you can save it:
  - File -> Save as preset (all fields different from default)
  - File -> Save as full preset (all input options)
- Load this: File -> Preset -> 'Your preset' on future jobs with the same setting

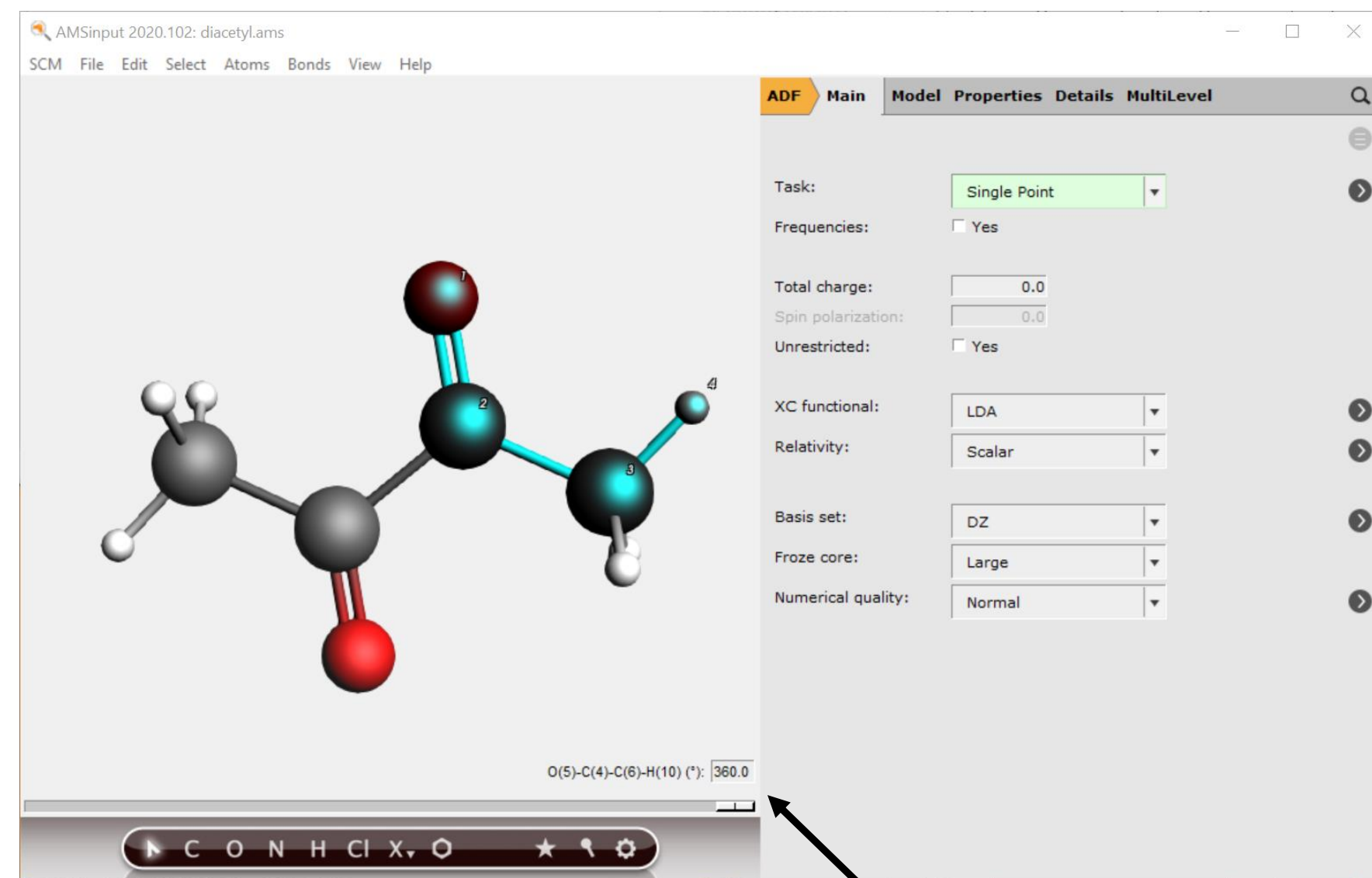
## 3. AMSprepare (& report)

- In amsjobs select a job, tools -> prepare
- Now you can run the same job but with different settings (e.g. basis set, xc, ... )
- With adfreport you can [build a report to visualize results](#) (e.g. distances)
- (also consider Python scripting with PLAMS)



# Building molecules (tutorials)

- Search molecules in GUI
- Import: InChI, SMILES, xyz, cif, pdb, ...
- Included structure library + building
- **Exercise:** Build diacetyl ( $C_4H_6O_2$ )
  - By searching for it in the GUI
  - By starting from the builder tools
    - use '2' for double bonds, Ctrl+E adds H's
  - By importing SMILES (e.g. from Wikipedia)
  - Select multiple atoms to change bond, angle, dihedral
- Symmetrize ( $C_{2h}$ ), pre-optimize (UFF, MOPAC, DFTB, MLPotential)
- Think about conformers!





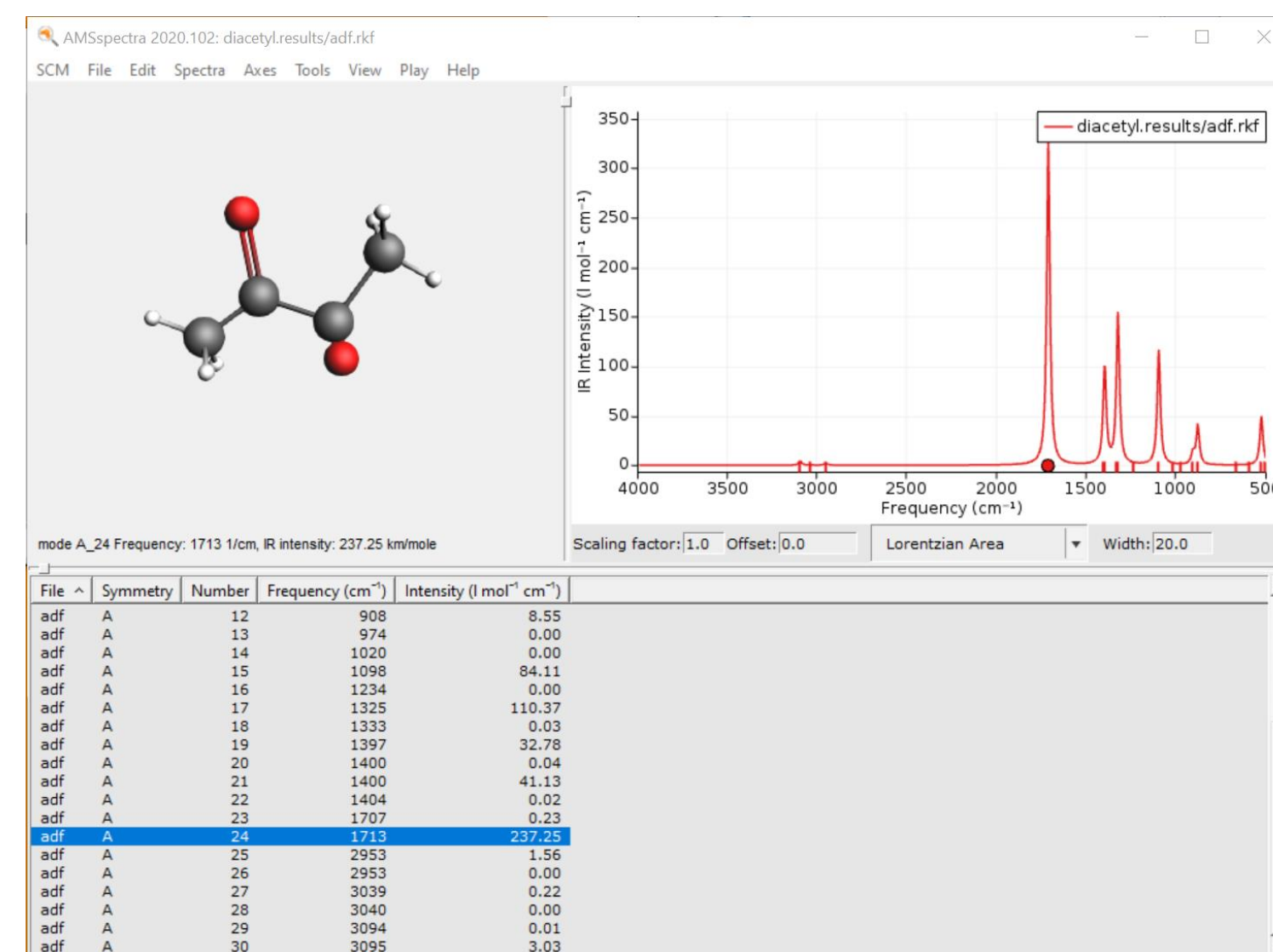
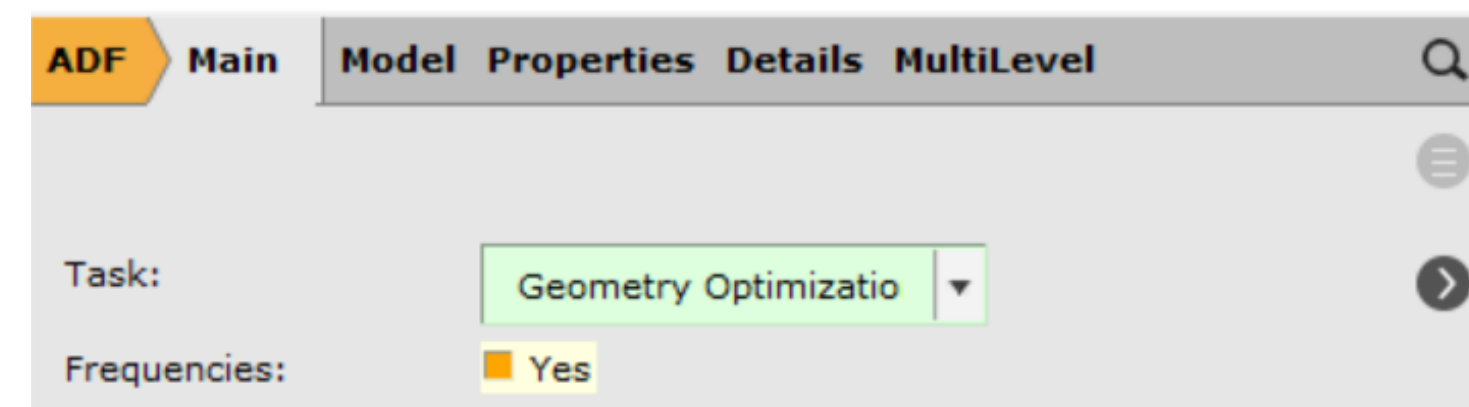
# Spectra: IR, other vibrational

- **Exercise:** Calculate & visualize frequencies

- Optimize geometry at same level as frequency calc.
- Task = Geometry Opt + Frequencies = Yes
- Try a few different methods:

- ADF: PBE-D4/DZP
- DFTB: DFTB3-D3-BJ/3ob-3-1
- MOPAC

- Visualize: AMSSpectra, animate some modes
- Axes-> Molar Absorption Coefficient
- Tweak broadening
- Compare to [NIST](#)
- Play with Spectra-> PVDOS



# Spectra: UV/VIS

- Exercise:

- With ADF: calculate 10 allowed excitations
  - use SAOP model potential, DZP (or TZP), no core
  - See also [UV/VIS FAQ for tips](#)
- Go to spectra, change x-axis to nm
- Increase the line width to ~10
- Visualize the pi-pi\* NTOs at ~205nm (click on NTO1)
- Visualize the MOs strongest Single Orbital Transition
- Compare to [NIST data](#) which peaks are missing?
  - Forbidden transitions? [Spin-orbit coupling?](#) [Vibronic?](#)
  - Check out
- More exercises
  - Rerun with method 'sTDA' and tick TDA
  - Also try TD-DFT+TB (ADF)
  - and TDDFTB ([DFTB3/3ob-3-1](#), [GFN-xTB](#) )
  - (can use the same PBE-D4 optimized geometry)

The screenshot shows the ADF software interface with the following settings:

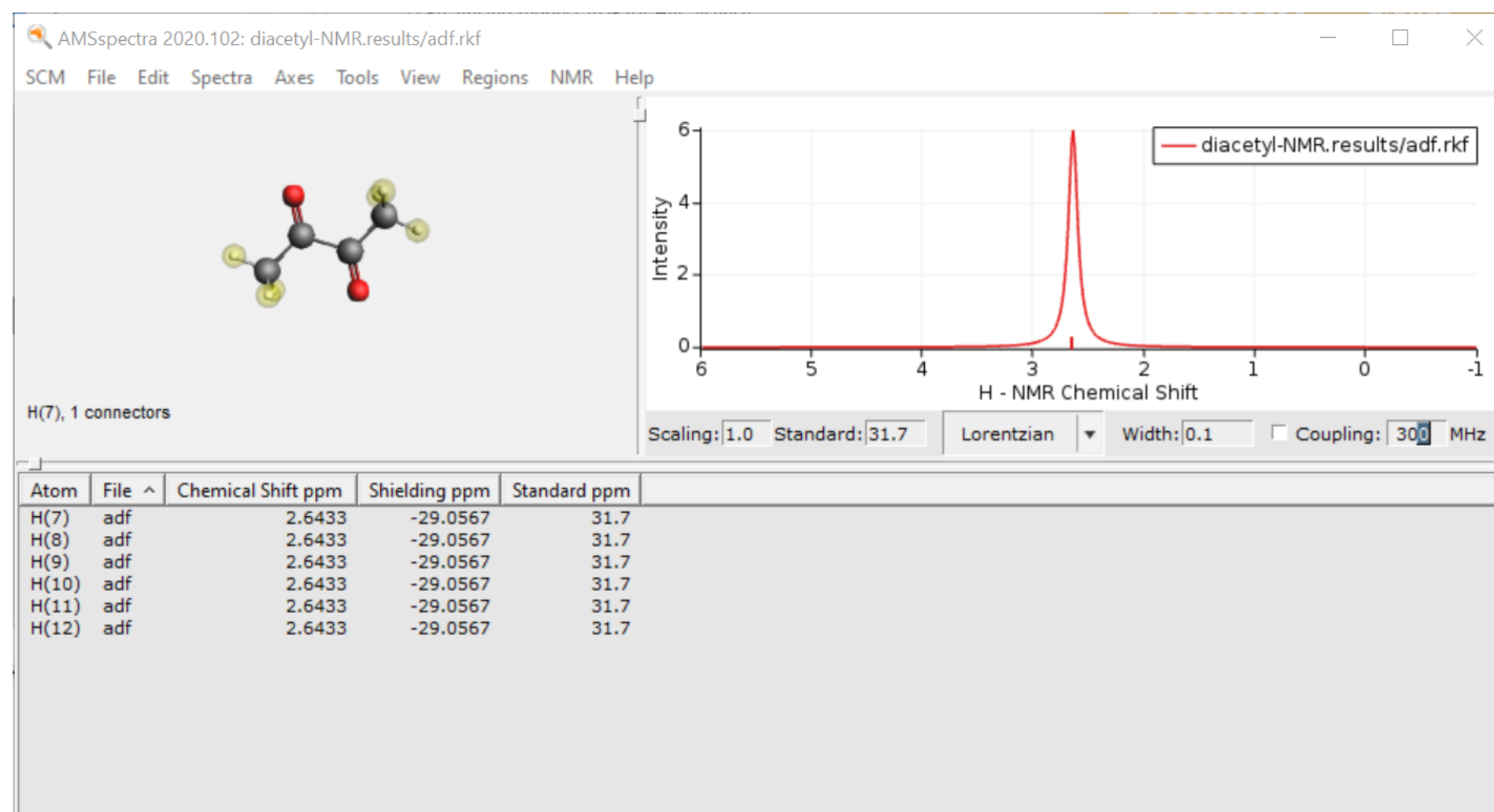
- Task: Single Point
- XC functional: Model:SAOP
- Relativity: Scalar
- Basis set: DZP
- Frozen core: None

The bottom panel is titled "Excitations (UV/Vis), CD" and contains the following settings:

- Type of excitations: AllowedOnly
- Method: Davidson
- TDA: ☐ Yes
- Number of excitations: 10

# Spectra: NMR

- Exercise:
  - See also [NMR FAQ for tips + advanced tutorials](#)
  - Use PBE0 + TZP, Scalar, no core
  - Select Properties -> NMR
    - select shielding for all H
  - Spectrum, NMR-> Chem. Equivalent regions
    - Note all H are equivalent (rotation), no coupling
  - Note the internal ref. uses different settings!
    - Recalculate TMS with same set up

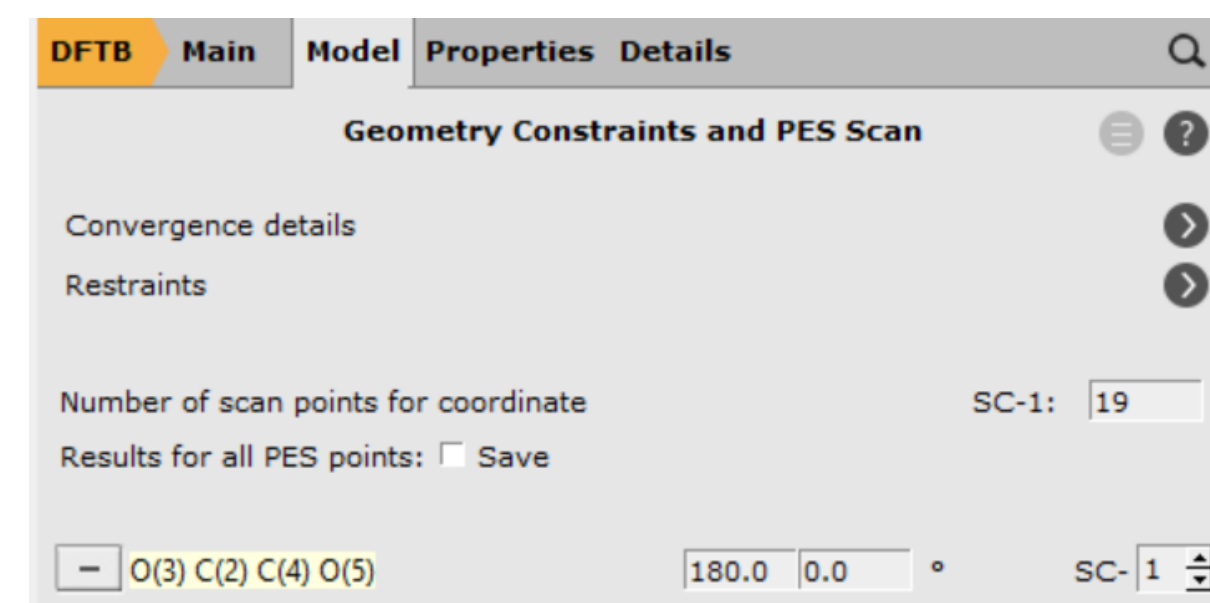
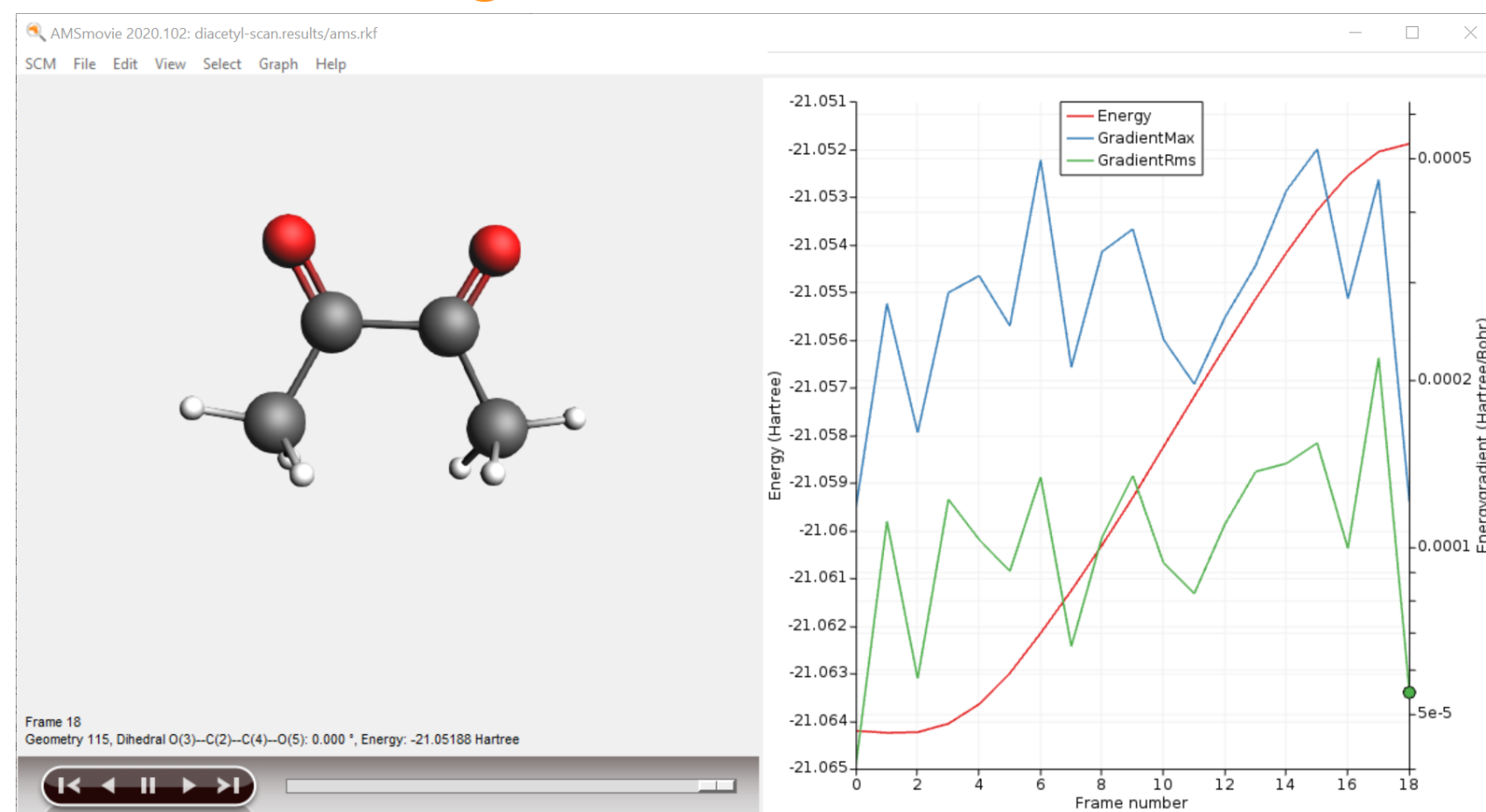




# PES: conformers, scan dihedral

- Exercises:

- Switch the engine to Conformers, run, visualize -> AMSMovie
  - Does it find all conformers :) ? Maybe try a larger molecule?
  - Switch to, e.g. DFTB, and from Model -> Coordinates, Use: Selected File, select your.sdf
  - Do a frequency run on all geometries and visualize a Boltzmann-averaged spectrum
- Take a DFTB input, set task to PES Scan, click >
  - Select dihedral and scan in 19 points from 180-0
  - Wait for calculation to finish -> AMSMovie
  - One can save geometries to start TS search (see later)



# Quick thermodynamic properties

- Exercise:

- Open SCM -> COSMO-RS
- In the SMILES input, put CC(=O)C(=O)C and Add
- Properties -> Pure compound
- Compare some properties (density, boiling point) (e.g. [Wikipedia](#))

Property		Unit
Boiling point	346.746	K
Critical pressure	51.21	bar
Critical temperature	524.603	K
Critical volume	0.195	L/mol
Liquid density	0.816	kg/L
Dielectric constant	10.985	
Absolute entropy (ideal gas)	309.848	J/(mol K)
Flash point	270.523	K
Gibbs energy of formation (ideal gas)	-111.468	kJ/mol
Net enthalpy of combustion	-1652.692	kJ/mol
Std. state enthalpy of formation	-188.906	kJ/mol
Enthalpy of fusion	17.129	kJ/mol
Enthalpy of formation (ideal gas)	-157.71	kJ/mol
Enthalpy of sublimation	49.534	kJ/mol
Melting point	213.82	K
Liquid molar volume	0.069	L/mol
Parachor	161.085	
Solubility parameter	10.098	$\sqrt{\text{MPa}}$
Triple point temperature	213.778	K
Van der Waals area	91.576	$\text{\AA}^2$
Van der Waals volume	63.229	$\text{\AA}^3$