

Tutorial 1: Command line and Lab 1



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Presentation agenda

- 1. Computer clusters
- 2. How to connect to a remote machine?
- 3. What is Terminal in Linux and how to work with it?
- 4. Avogadro editor
- 5. Some reminders on semi-empirical methods
- 6. MOPAC program. Technical aspects
- 7. Lab 1 overview

What is a cluster for computing tasks?





(compare this with a 1988 Cray YMP/8 at 2.7 GF/s)



Compute Chip

2 processors

2.8/5.6 GF/s

4 MiB* eDRAM

Compute Card or I/O Card

FRU (field replaceable unit) 25 mm x 32 mm 2 nodes (4 CPUs) $(2 \times 1 \times 1)$ 2 x (2.8/5.6) GF/s 2 x 512 MiB* DDR 15 W

Node Card

16 compute cards 0-2 I/O cards 32 nodes (64 CPUs) $(4 \times 4 \times 2)$ 90/180 GF/s 16 GiB* DDR 500 W

Cabinet

2 midplanes 1024 nodes (2,048 CPUs) (8 x 8 x 16) 2.9/5.7 TF/s 512 GiB* DDR 15-20 kW

* http://physics.nist.gov/cuu/Units/binary.html

Skoltech

64 cabinets 65,536 nodes (131,072 CPUs) (32 x 32 x 64) 180/360 TF/s 32 TiB* 1.5 MW 2,500 sq.ft. MTBF 6.16 Days

System



Settings for your laptop

How to connect to Virtual Machine (cluster) via SSH?

Windows: via <u>PuTTY</u> (portable version is enough)

'your_login'@10.30.16.180 'your password'

8 - 0	PuTTY Configuration			
Category: • Session Logging	Basic options for your Specify the destination you want to Host <u>Name</u> (or IP address)	PuTTY sess connect to	ion Port	
 Terminal 	a.boev@10.30.16.180		22	
Keyboard Bell	Connection type: O Raw O Telnet O Rlogin	0 <u>S</u> SH	○ Se <u>r</u> ial	
Features - Window Appearance	Load, save or delete a stored session Sav <u>e</u> d Sessions	חס		
Behaviour Translation	Default Settings		Load	
Selection			Sa <u>v</u> e	
Fonts • Connection			<u>D</u> elete	
Data Proxy Telnet Blogin	Close window on e <u>x</u> it: O Always O Never O	Only on clea	in exit	
About		Open	Cancel	

Linux/Mac: via Terminal

ssh 'your_login'@10.30.16.180 'your_password'



port 25

How to copy files b/t laptop and VM?

Windows: via WinSCP

'your_login'@10.30.16.180 'your_password'

Y New Site	Session	
	File protocol:	
	SCP	\sim
	Host name:	Port number:
	genuse50.smu.edu	22
	User name:	Password:
	testg	•••••
	Save <	Advanced

Linux/Mac: via Terminal

scp -r 'your_local_file' 'your_login'@10.30.16.180:'path_to_folder_on_VM'



An alternative for Windows: Mobaxterm

SSH session with terminal:

Terr	ninal	Sessions	View	X server	Tools	Games	Settings	Macros	Help
Q	uick	connect.	**				2. /home/m	obaxterm	
🍝 Tools 🗡 Sessions 🔌		Iser sessions Iser sessions AIX Serve Linux Des Linux Lap Linux Ser Mac Com My Virtua PuTTY set	ers sktops otops vers puters al Machine	s	[20]	12-06-2	(X ser X11-For SSH-Age Active Active X11 dis	MobaXt ver, SS warding nt: SSH tun service play:	erm H cl : nels s:
🔪 Macros		 Solaris Se Windows Windows Windows Windows MySatelli 	ervers Desktops Laptops Servers te				10003		

Transferring files from your PC on the remote cluster; Transferring files from one directory to another on the remote machine.





Midnight commander (MC) file manager



		anton@k	omp: ~		×	<u></u>	mc [a	i.bo	ev@ces
Left	File	Command	Options	Right					
Left 'n / /Lab1 /abinit /abinit /bin /fhiaims /gaussia /gaussia /gaussia	File test	anton@k	omp: ~ Options Name	Right		Size UPDIR 66 63 185 42 92 50 38 22	mc [a Modi Oct Oct Nov Nov Nov Dec Oct Nov Oct	i.bo 19 12 7 27 28 7 29	ev@ces .[^]> time 16:51 17:53 2019 2019 2018 2019 2021 2021 2018 2019 2021 2018 2019
/gulp.te /lammps	est					77 56	Nov Oct	26 29	2018 2019
/lammps. /mopac /mopac.t	test					128 54 54	Nov Oct Oct	7 27 27	2018 11:13 17:35
/public /uspex /uspex.t	tést					6 39 4096	Dec Dec Dec	27 11 11	2019 2019 2019
/vasp /vasp.te	est					266 308	Oct Nov	28 7	2021 2018
test.ou	1.tgz Jt					1382 26248K 141	Oct Oct	27 26 27	2019 2020 11:12

Hotkeys in MC

• **TAB** – switch active panel. • *F*<1-10>



Ctrl+O – switch between MC window and command line.

• F3/F4 - read only/edit mode

Left File Command Options Right					1 POSCAP [] 0 · [1-
<pre>~/vasp/surseg_tem/seg_paper/slab/LC.104.m05.7l.1U</pre>	LC_g		1942-0	[^]> ₁	
'n Name	Size	Modi	ify	time	2a=[Co,Li,O] ; LC.104.22W.8.1.end
1	UPDIR	ОКТ	27	11:12	1.00000000000000
1.CHGCAR.gz	82407K	OKT	2	09:07	11.348340 0.000000 -0.530610
1.CONTCAR	24954	окт	2	09:05	0 004760 44 470444 0 740440
1.OUTCAR	30373K	окт	2	09:06	-0.034/00 11.4/8141 -0./43419
1.POSCAR	14516	OKT	1	12:47	0.000000 0.000000 30.405135
EIGENVAL	45032	окт	2	09:06	ColiO
IBZKPT	132	окт	2	01:03	
INCAR	1050	окт	1	12:47	56 56 112.
KPOINTS	37	ОКТ	1	12:47	Direct
LC.104.m05.7l.1ULC_g.1.log	29608	окт	2	09:06	0 0533031256806230 0 1880702840
*LC.104.m05.7l.1ULC_g.run	843	окт	1	12:47	0.05555551250050255 0.100575204
POSCAR	14516	окт	2	01:03	0.5533931256896238 0.1889792849
POTCAR	484219	окт	1	12:47	0.0533931256896238 0.6889792849
sbatch.err	/9	OKT	2	09:07	0.5533931256896237 0.6889792849
Spacen.ouc	0	OKI	2	01.05	0 3033031256806238 0 1880702840
					0.3033331230030230 0.100373204
					0.8033931256896238 0.1889792849
					0.3033931256896238 0.6889792849

Open file in MC

Skoltech

0.96 0.96 0.96 0.96 0.96 0.969

1/233]

0

An alternative for Linux: Termius

SSH sessions with terminal:



Transferring files from your PC on the remote cluster; Transferring files from one directory to another on the remote machine.

puref >	Downloads	Q Filter	Actions ✓	 ccmm ccmm home > a.burov > 	lab1	Q Filter	- ,* × Actions ∨
	Date Modified	Size	Kind	Name	Date Modified	Size	Kind
	10/1/2020, 11:59 PM		folder	· · ·			
	9/12/2023, 2:16 PM	275.27 kB	pdf	Lab1_benzene	11/3/2023, 3:21 PM		folder
	10/12/2023, 1:52 AM	2.15 kB	POSCAR	Lab1_benzene.zip	10/31/2022, 1:59 AM	1.27 MB	zip
		733.00 Bytes	CONTCAR	Lab1.pdf	10/31/2022, 1:59 AM	77.77 kB	pdf
	10/24/2023, 11:21 PM	1.09 MB	txt	-rw-rw-r			





550 x 318

http://jmol.sourceforge.net/

How to visualize atoms?







Jmol supports lots of structure file formats (~100)

The most commonly used are XYZ and Crystallographic Information File (cif) formats.

24			
Caff	eine		
Н	-3.3804130	-1.1272367	0.5733036
N	0.9668296	-1.0737425	-0.8198227
С	0.0567293	0.8527195	0.3923156
N	-1.3751742	-1.0212243	-0.0570552
C	-1.2615018	0.2590713	0.5234135
C	-0.3068337	-1.6836331	-0.7169344
C	1.1394235	0.1874122	-0.2700900
N	0.5602627	2.0839095	0.8251589
0	-0.4926797	-2.8180554	-1.2094732
C	-2.6328073	-1.7303959	-0.0060953
0	-2.2301338	0.7988624	1.0899730
н	2.5496990	2.9734977	0.6229590
C	2.0527432	-1.7360887	-1.4931279
Н	-2.4807715	-2.7269528	0.4882631
н	-3.0089039	-1.9025254	-1.0498023
Н	2.9176101	-1.8481516	-0.7857866
н	2.3787863	-1.1211917	-2.3743655
н	1.7189877	-2.7489920	-1.8439205
C	-0.1518450	3.0970046	1.5348347
C	1.8934096	2.1181245	0.4193193
N	2.2861252	0.9968439	-0.2440298
н	-0.1687028	4.0436553	0.9301094
н	0.3535322	3.2979060	2.5177747
Н	-1.2074498	2.7537592	1.7203047

1	<pre># generated using pymatgen</pre>
2	data LiCoO2
3	<pre>symmetry_space_group_name_H-M 'P 1'</pre>
4	_cell_length_a 2.84289827
5	cell length b 2.84289827
6	cell length c 14.14561550
7	cell angle alpha 90.00000000
8	cell angle beta 90.00000000
9	cell angle gamma 120.00000000
10	loop
11	atom site type symbol
12	atom site label
13	atom site symmetry multiplicity
14	atom site fract x
15	atom site fract y
16	atom site fract z
17	atom site occupancy
18	Li Li0 1 0.0000000 0.0000000 0
19	Li Lil 1 0.666666667 0.33333333 0
20	Li Li2 1 0.33333333 0.666666667 0
21	Co Co3 1 0.33333333 0.666666667 0
22	Co Co4 1 0.0000000 0.0000000 0
23	Co Co5 1 0.666666667 0.333333333 0
24	0 06 1 0.0000000 0.0000000 0.2
25	0 07 1 0.666666667 0.333333333 0.0
26	0 08 1 0.666666667 0.33333333 0.5
27	0 09 1 0.33333333 0.666666667 0.4
28	0 010 1 0.33333333 0.666666667 0.
29	0 011 1 0.0000000 0.0000000 0.

(~100) if) formats.



Command line basics

What is the Terminal in Linux?

The **terminal** is the GUI window that you see on the screen. It takes commands and shows output.

The **shell** is the software that interprets and executes the various commands that we type in the terminal.

Bash is a particular shell. It stands for Bourne Again
Shell.





Basic bash commands

- Is show the content of the current directory
- *cd* <directory> change directory
- cd .. change current directory to parent directory
- *pwd* show the path to the current directory
- *touch* <name.ext> create a new file with extension .ext
- *mkdir* <name> create a new directory
- *rm* <name.ext> remove file
- **rm -r** <name> remove the directory
- *cat* <file> show a file

Cheat sheet with Linux commands



List of useful terminal commands

- ssh username@10.30.16.180 access to the cluster
- *mc* run file manager
- Ctrl+O switch between MC and command line
- **Tab** switch between MC panels (left right)
- squeue show job schedule on cluster
- *unzip name.zip* unzip archive
- *zip -r <name of new archive>.zip <folder name> compress a folder* into zip archive

Cheat sheet with Linux commands 17



Construction of molecules (Avogadro)





offers flexible high quality rendering and a powerful plugin architecture.

<u>File Edit View Buil</u>	d <u>S</u> elect <u>C</u>	rystal	<u>Extensions</u>	Quantum H	elp
New 📔 Open	Close	🕗 Sav	e 🔯 Save	As 🖹 Mole	cule 🛛 🔶 🔦
Measure		0× *			
Display Types		Ø×			
V Ball and Stick					
Van der Waals					
Wireframe					
Force					
✓ Meshes	-				
Van der Waals (AO)	entay				
View Configuration	Display Ty				
Malagulas					
Molecules	*				
oncicie (contra)					
				-	
		Г	istance	4 41905	Å
			2000000	1,11000	

Avogadro editor

Avogadro is an advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It





Molecules





Avogadro can build:

Nanotubes

DNA/RNA



A little of theoretical information

Some images are taken from: http://openmopac.net/

Semi-empirical methods

Ignore core electrons: only consider valence electrons Replace many costly two-electron integrals in HF theory with parameters

Parameters from experimental and high-level calculations Good parameters can give solutions with accuracy of HF theory

DFT and post-HF methods include more electron correlation, so are more accurate

Semi-empirical good for:

- Quick geometry screening **Big systems before DFT**
- **Compromise:** properties instead of DFT for big molecules

Semi-empirical bad for:

- Heavy atoms Transition metals (generally)
- **Open-shell systems**
- Small systems (DFT cheap) (Intermolecular interactions)

AM1 (Austin) RM1 (Recife) PM6 (Parameterisation) PM7 ZINDO/S (Zerner's intermediate neglect of differential overlap) (Hyperchem)

Earliest model

Good for organics

Bad for geometries

MOPAC. Parameterizations

- Superseded by PM3 (then 6,7)
- Lacks heavier atoms (e.g. Si)
- Heavily parameterised model. Wide applicability. Includes TMs Has dispersion and H-bond optimised versions
- Bad for sp2 nitrogen planarity
- Improvement on PM6
- Nitrogens in amino acids still bad
- Good for electronic spectra: may beat B3LYP in many cases!
- Often good to add empirical parameters for π and s overlap.





Semi-empirical methods



	522	S66x8	X40	WATERI	17	S30L	S30Ln	K23
PBE-D3/'CBS'	0.6	0.4	0.5	1.3	2.0	6.6	4.7	1.
HF-3c	0.6	0.4	1.4	1.1	1.2	6.5	4.0	2.3
HF-3cv	1.7	0.5	2.1	2.3	2.4	7.4	5.3	3.
DFTB3-D3	1.0	0.8	1.8	0.4	1.7	6.2	3.6	2.
OM2-D3	0.9	0.8	-	0.9	2.9	6.7	3.7	-
PM6-D3H4X	0.7	0.5	1.2	0.7	2.9	6.7	4.8	-
PM6-D3H+	0.6	0.6	1.5	1.6	2.6	6.2	4.6	-
MSINDO-D3H+	1.5	1.1	1.4	1.5	5.7	9.5	8.8	6.0
PM7	0.8	0.7	1.8	0.5	6.5	16	11	
MAD / kcal·mol ⁻¹	1							



MOPAC manual

MOPAC (Molecular Orbital PACkage) is a semiempirical quantum chemistry program. Semiempirical methods contain sets of parameters.

Parameter	Description	Units	MNDO	AM1	PM3	
$\mathbf{U}_{ss}, \mathbf{U}_{pp}, \mathbf{U}_{dd}$	s, p, and d atomic orbital one-electron one-center integrals	eV	*	*	*	
$\beta_s, \beta_p, \text{ and } \beta_d$	s, p, and d atomic orbital one-electron two-center resonance integral terms	eV	*	*	*	
$\xi_s, \xi_p, \text{ and } \xi_d$	s, p, and d Slater atomic orbital exponent	bohr ⁻¹	*	*	*	
$\xi_{sn}, \xi_{pn}, \text{ and } \xi_{dn}$	s, p, and d Slater atomic orbital internal exponent	bohr ⁻¹	*	*	*	
a _A	Atom A core-core repulsion term	Å ⁻¹	*	*	*	
a.AB	Atoms A and B core-core repulsion term	Å ⁻¹				

MOPAC

Table of Parameters





A little of technical information



MOPAC: Input file

Input file: water.mop



water.arc Archive file: job results and final coords

water.out Output log file: shows calculation input, progress, results and errors

water.res

Restart file: written for long jobs; can restart job by passing "restart" command in original job input file

water.end

This file is empty. If you put text into it, MOPAC will save restart and density files and will stop the calculation

water.den Density file: contains density matrix You'll never need this

water.mgf Generated with GRAPHF keyword, and gives orbitals which can be viewed in Jmol.

water.aux

Generated with AUX keyword. Gives extra info which can be viewed with some visualisers (e.g. GABedit)

MOPAC: Input file

'Method' 'Some parameters' 'User comments' 'Empty string' Geometry*

*Each line starts with the atomic symbol, followed by x,y,z coordinates. Whether these parameters are variables or constants during the geometry optimization is indicated by a trailing 0 (constant) or 1 (variable).

PM	GNORM=0) -in	nization
GCON	leciy opt	•+"	
С	1.397	1	0
C	0.6985	1	1.20983749
C	-0.6985	1	1.20983749
C	-1.397	1	0
C	-0.6985	1	-1.20983749
C	0.6985	1	-1.20983749
Н	2.481	1	0
H	1.2405	1	2.14860903
Н	-1.2405	1	2.14860903
H	-2.481	1	0
Н	-1.2405	1	-2.14860903
Н	1.2405	1	-2.14860903



MOPAC: Methods used in the Lab 1

- PM7 uses a "D2" type correction for the elements: H, He, B, C, N, O, F, Ne, P, S, Cl, Ar, Br, and Kr. For the other elements, a core-core Gaussian attractive terms is used to mimic dispersion. This means that some form of dispersion is present for all elements. The core-core Gaussian terms are optimized to reproduce reference geometries and heats of formation.
- The best method for general chemistry, and for solids. Optimized to reproduce the Standard Heat of Formation, ΔH_{f} .
- Perfectly fits for inorganic solids.

PM7 is the Modified Neglect of Diatomic Overlap, Parametric Method Number 7



Lab 1 practice



1. Geometry optimization

1	P	M7 GNORM=0)		
2	Ge	ometry opt	:ir	nization	
3					
4	С	1.397	1	0	1
5	С	0.6985	1	1.20983749	1
6	С	-0.6985	1	1.20983749	1
7	С	-1.397	1	0	1
8	С	-0.6985	1	-1.20983749	1
9	С	0.6985	1	-1.20983749	1
10	Η	2.481	1	0	1
11	H	1.2405	1	2.14860903	1
12	Η	-1.2405	1	2.14860903	1
13	H	-2.481	1	0	1
14	Η	-1.2405	1	-2.14860903	1
15	Η	1.2405	1	-2.14860903	1

.mop extension molec_PM7_em.mop [a.boev@cest-cms-ccmm Lab1_benzene]\$ mopac molec_PM7_em.mop

<u>GNORM</u> is geometry optimization termination criteria. Allows the geometry optimization to exit as soon as the gradient norm dropped below 0.01 kcal/mol/Ångstrom





1. Geometry optimization

molec_PM7_em.out

FINAL	HEAT	OF	FORM	ATION	=		22.	95	542	KC	AL/
COSMO	AREA				=		119	70	SQ	UAR	EA
COSMO	VOLU	ME			=		108.	36	CU	BIC	AN
GRADI	ENT N	ORM			=		0.	006	597		
IONIZ	ATION	POT	ENTI	AL	=		9.	824	405	7 E	V
HOMO	LUMO	ENEF	GIES	(EV)	=		-9.	824	4 (0.2	36
NO. 0	F FIL	LED	LEVE	LS	=		15				
MOLEC	ULAR I	WEIG	GHT		=		78.	113	34		
MOLEC	ular i	DIME	NSIO	NS (Ar	ngstrom	s)					
Ato	m	ŀ	tom		Distan	ce					
Н	12	H	ł	9	4.963	76					
Н	10	H	ł	7	4.298	70					
Н	8	(4	0.000	00					
SCF C	ALCUL	ATIC	ONS		=		17				
WALL-	CLOCK	TIM	1E		=	0.	070	SEC	CONI	DS	
COMPU	TATIO	N TI	ME		=	0.	095	SEC	CON	DS	

/MOL = 96.04546 KJ/MOL

ANGSTROMS

= 0.00201 PER ATOM

POINT GROUP: D6h



1	AU	X(MOS=0, PRECISIC)N=4)	PM7	FORCE	
2	Vib	rations				
3						
4	С	1.39399329	1	0	00000000	1
5	C	0.69699665	1	1.	20723360	1
6	С	-0.69699665	1	1.	20723360	1
7	C	-1.39399329	1	0.	00000000	1
8	С	-0.69699665	1	-1.	20723360	1
9	С	0.69699665	1	- 1 .	20723360	1
LO	Н	2.48186046	1	0	00000000	1
11	Н	1.24093023	1	2.	14935421	1
12	H	-1.24093023	1	2.	14935421	1
13	Н	-2.48186046	1	0	00000000	1
14	Н	-1.24093023	1	- 2 .	14935421	1
15	H	1.24093023	1	- 2	14935421	1

molec_PM7_freq.mop

2. Vibrational frequency calculation



FORCE – shows the force constants for the molecule.

- 22.956501 KCALS/MOLE HEAT OF FORMATION =
- 60.211 KCAL/MOL ZERO POINT ENERGY

NORMAL COORDINATE ANALYSIS (Total motion = 1 Angstrom)

Root No.	1	2	3	4
	1 E2u	1 E2u	1 B1g	1 E2g
	346.1	346.1	592.1	600.3

2. Vibrational frequency calculation

5	6	7	8
1 E2g	1 A2u	1 E1g	1 E1g
600.3	757.3	900.2	900.2

DESCRIPTION OF VIBRATIONS

VIBRATION	2 1E2u	ATOM PAIR	ENERGY CONTRI
FREQUENCY	346.12	C 2 C 3	+22.7% (1
TRANSITION DIPOLE	0.0000	C 5 C 6	+22.7% (1
TRAVEL (Ang.)	0.4069	C 3 C 4	+13.5% (
REDUCED MASS	1.1769	C 1 C 6	+13.5% (
EFFECTIVE MASS	18.7542		
FORCE CONSTANT	0.0831		
VIBRATION	3 1B1g	ATOM PAIR	ENERGY CONTRI
FREQUENCY	502 06	C 1 C 5	+13 1% (
	592.00	C 4 C J	113.1/0 (
TRANSITION DIPOLE	0.0000	C 5 C 6	+13.1% (
TRANSITION DIPOLE TRAVEL (Ang.)	0.0000	C 5 C 6 C 1 C 6	+13.1% (
TRANSITION DIPOLE TRAVEL (Ang.) REDUCED MASS	0.0000 0.4437 0.5786	C = 4 = - C = 3 C = 5 C = 6 C = 1 C = 6 C = 3 C = 4	+13.1% (+13.1% (+13.1% (
TRANSITION DIPOLE TRAVEL (Ang.) REDUCED MASS EFFECTIVE MASS	0.0000 0.4437 0.5786 10.0031	C = 4 = - C = 3 C = 5 C = 6 C = 3 C = 4 C = 1 C = 2	+13.1% (+13.1% (+13.1% (+13.1% (
TRANSITION DIPOLE TRAVEL (Ang.) REDUCED MASS EFFECTIVE MASS FORCE CONSTANT	0.0000 0.4437 0.5786 10.0031 0.1195	$\begin{array}{c} C & 4 & & C & 3 \\ C & 5 & & C & 6 \\ C & 1 & & C & 6 \\ C & 3 & & C & 4 \\ C & 1 & & C & 2 \\ C & 2 & & C & 3 \end{array}$	+13.1% (+13.1% (+13.1% (+13.1% (+13.1% (

- IBUTION 49.8%) 49.8%) 49.8%) 49.8%) 49.8%) 0.0% 49.8%)
- RADIAL 0.0% 0.0% 0.0% 0.0% 0.0%
- 0.0% 10.3%) 0.0% 0.0% 85.0%) 0.0% 85.0%)
- RADIAL IBUTION 10.3%)

3. Single point calculation

1	GRAPH	F PM7 1SCF A	LLVEC	AUX (MOS=99999	9,P
2	Single	point			
3					
4	С	1.39399329	1	0.00000000	1
5	С	0.69699665	1	1.20723360	1
6	С	-0.69699665	1	1.20723360	1
7	С	-1.39399329	1	0.00000000	1
8	С	-0.69699665	1	-1.20723360	1
9	С	0.69699665	1	-1.20723360	1
LO	Н	2.48186046	1	0.00000000	1
11	Н	1.24093023	1	2.14935421	1
12	Н	-1.24093023	1	2.14935421	1
L3	Н	-2.48186046	1	0.00000000	1
L4	Η	-1.24093023	1	-2.14935421	1
L5	Н	1.24093023	1	-2.14935421	1
March 1999					

molec_PM7_sp.mop

PRECISION=4)

0.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.000000001

<u>**GRAPHF**</u> – writes a formatted file, <name>.mgf with the Information about Molecular Orbitals, which can be visualized with Jmol program.

<u>1SCF</u> – is a single SCF calculation of a geometry.

ALLVEC – allows printing of all the MO into the output file.

3. Single point calculation

Jmol \rightarrow molec_PM7_sp.mgf \rightarrow RButton \rightarrow Surfaces \rightarrow Molecular Orbitals

HOMO: -9.82 eV (Doubly generated) LUMO: 0.24 eV (Doubly generated)



4. Localized Molecular orbitals

1	GR/	APHF AUX(MOS=999	999	PRECISION=4) PM7	19
2	Loca	alized MO			
3					
4	C	1.39399329	1	0.00000000 1	
5	C	0.69699665	1	1.20723360 1	
6	C	-0.69699665	1	1.20723360 1	
7	C	-1.39399329	1	0.00000000 1	
8	C	-0.69699665	1	-1.20723360 1	
9	C	0.69699665	1	-1.20723360 1	
10	Н	2.48186046	1	0.00000000 1	
11	Н	1.24093023	1	2.14935421 1	
12	Η	-1.24093023	1	2.14935421 1	
13	Н	-2.48186046	1	0.00000000 1	
14	Η	-1.24093023	1	-2.14935421 1	
15	H	1.24093023	1	-2.14935421 1	

molec_PM7_Imo.mop

LOCALIZE ALLVEC SCF

0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1
0.00000000	1

FORCE – gives the force constants for the molecule.

LOCALIZE – prints the occupied eigenvectors as transformed into a localized in the output file.

4. Localized Molecular orbitals

C-C σ-bond (-19.94 eV)



molec_PM7_Imo.out

C-H σ-bond (-17.56 eV)



5. Triplet geometry optimization

PM	7 UHF TRIPLET G	NORM=0							
То	get correctly o	riented	molecule we	e slight	ly expanded	d C2-C3	and C	5-C6	bonds
С	1.39399358	1	0.00000000	1	0.00000000	1			
C	0.71699679	1	1.20723386	1	0.00000000	1			
С	-0.71699679	1	1.20723386	1	0.00000000	1			
C	-1.39399358	1 -	0.00000000	1	0.00000000	1			
С	-0.71699679	1 -	1.20723386	1	0.00000000	1			
С	0.71699679	1 -	1.20723386	1	0.00000000	1			
Н	2.48186088	1	0.00000000	1	0.00000000	1			
H	1.24093044	1	2.14935457	1	0.00000000	1			
Н	-1.24093044	1	2.14935457	1	0.00000000	1			
H	-2.48186088	1	0.00000000	1	0.00000000	1			
Н	-1.24093044	1 -	2.14935457	1	0.00000000	1			
H	1.24093044	1 -	2.14935457	1	0.00000000	1			

molec_T_PM7_em.mop

Ε

Singlet No unpaired e**<u>UHF</u>** – the unrestricted Hartree-Fock Hamiltonian is to be used.

TRIPLET – triplet state is defined.

<u>GNORM</u> – geometry optimization stop criterion. Allows the geometry optimization to exit as soon as the gradient norm dropped below 0.01 kcal/mol/Ångstrom.



Doublet 1 unpaired e-

Triplet 2 unpaired e-

5. Triplet geometry optimization

FINAL HEAT OF FORMATION =

COSMO AREA	=
COSMO VOLUME	=
GRADIENT NORM	=
IONIZATION POTENTIAL	=
ALPHA SOMO LUMO (EV)	=
BETA SOMO LUMO (EV)	=
NO. OF ALPHA ELECTRONS	=
NO. OF BETA ELECTRONS	=
MOLECULAR WEIGHT	=

C2–C3 and C5–C6 bonds are elongated to 1.482 A and other bonds are compressed to 1.386 A.

76.82977 KCAL/MOL = 321.45576 KJ/MOL 119.88 SQUARE ANGSTROMS 108.45 CUBIC ANGSTROMS 0.00175 PER ATOM 0.00607 = 7.393328 EV -7.393 0.656 -10.311 -2.048 16 14 78.1134 POINT GROUP: D2h

6. Triplet Vibrational frequency calculation

1	AU	X(MOS=0,PRECISIO)N=4)	PM7	UHF	TRIP
2	Vib	rations				
3						
4	С	1.42788504	1	0.	0000	00000
5	С	0.74084873	1	1.	2034	0293
6	С	-0.74084873	1	1.	2034	0293
7	С	-1.42788504	1	0.	0000	00000
8	С	-0.74084873	1	-1.	2034	0293
9	С	0.74084873	1	-1.	2034	0293
10	H	2.51842877	1	0.	0000	00000
11	H	1.24433052	1	2.	1578	30940
12	Η	-1.24433052	1	2.	1578	30940
13	H	-2.51842877	1	0.	0000	00000
14	Η	-1.24433052	1	-2.	1578	30940
15	H	1.24433052	1	-2.	1578	30940

molec_T_PM7_freq.mop



UHF – the unrestricted Hartree-Fock Hamiltonian is to be used.

TRIPLET – triplet state is defined.

FORCE – gives the force constants for the molecule.



6. Triplet Vibrational frequency calculation

76.829766 KCALS/MOLE HEAT OF FORMATION =

ZERO POINT ENERGY 56.229 KCAL/MOL

NORMAL COORDINATE ANALYSIS (Total motion = 1 Angstrom)

Root No.	1	2	3	4	5	6	7	8
	1 Au	1 B2g	1 B3u	1 B3g	1 Ag	2 B3u	1 B1g	2 B2g
	103.7	232.4	297.5	501.4	575.9	670.0	741.0	779.2



7. Triplet Single point calculation

1	GRAPH	F PM7	UHF	TRI	IPLET	1SCF	ALLVEC	AUX (M
2	Single	point						
3								
4	C	1.42	27885	504	1	0.0	0000000) 1
5	C	0.74	10848	373	1	1.2	20340293	31
6	C	-0.74	10848	373	1	1.2	20340293	31
7	C	-1.42	27885	504	1	0.0	00000000	0 1
8	C	-0.74	10848	373	1	-1.2	20340293	31
9	С	0.74	10848	373	1	-1.2	20340293	31
10	Н	2.51	8428	377	1	0.0	0000000) 1
11	H	1.24	4330	952	1	2.1	15780940) 1
12	H	-1.24	4330	952	1	2.1	15780940	0 1
13	H	-2.51	8428	377	1	0.0	00000000) 1
14	H	-1.24	4330	952	1	-2.1	15780940	0 1
15	H	1.24	4330	952	1	-2.1	15780940	\mathbf{D} 1

molec_T_PM7_sp.mop

10S=99999, PRECISION=4) 0.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.0000000010.000000001

<u>GRAPHF</u> – writes a formatted file, <name>.mgf with the Information about Molecular Orbitals needed by Jmol program.

<u>1SCF</u> – is a single SCF calculation of a geometry.

ALLVEC – allows printing of all the MO into output file.

UHF – the unrestricted Hartree-Fock Hamiltonian is to be used.

TRIPLET – triplet state is defined.

7. Triplet Single point calculation

 $Jmol \rightarrow molec_T_PM7_sp.mgf \rightarrow RButton \rightarrow Surfaces \rightarrow Molecular \ Orbitals$

α

SOMO: -7.39 eV

LUMO: -2.05 eV



SOMO is singly occupied MO

ß eV SOMO: -10.31 eV LUM

LUMO: 0.65 eV

Parameters for advances calculations: Full list of parameters

Eigenvalues – units of eV; **Frequencies** – units of cm⁻¹.

its elements, with everything being in its standard state.

ITER – shows information on SCF.

COSMO area (COnductor-like Screening MOdel) – <u>model for solvation</u>. FINAL HEAT OF FORMATION – relative to elements in standard states.

<u>CHARGE</u> – Used to calculate properties of ions and specifies system charge.

- **GRADIENT NORM** kcal/mol/Angstrom multiply by 43.37 to get eV/Ångstrom, 0.01 kcal/mol/Ångstrom = 0.4 meV/A.
- Heat of Formation (ΔH_{f}) the change in enthalpy, in kcal mol⁻¹ or kj mol⁻¹, when one mole of a system is formed from

- **IONIZATION POTENTIAL Vertical IP = HOMO** according to the **Koopman's theorem**.
- **DIPOLE POINT-CHG. vs HYBRID** different methods to calculate dipole charge. For more details, look in the manual.









