User's Manual

`molSimplify` version 1.0

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1 General information

molSimplify is an open source utility that incorporates geometric manipulation routines necessary for the generation of transition metal complexes,automated setup and completion of electronic structure calculations, post-processing and data analysis. The software generates a variety of coordination complexes with any number of metals coordinated by ligands in a single or multidentate (chelating) fashion. The code can both build the coordination complex starting from a single metal atom or work to functionalize a more complex structure (e.g. a porphyrin or other metal-ligand complex) by including additional ligands or replacing existing ones. molSimplify builds intermolecular complexes for evaluating binding interactions and generating candidate reactants and intermediates for catalyst reaction mechanism screening and also supports interaction with chemical databases. Furthermore, it provides a Graphical User Interface (GUI) and is thus accessible to a wider audience since it does not require a lot of prior computational chemistry experience.

2 Installation

2.1 From source

2.2 Binaries

- installation multiwfn
- installation databases (links and how to install etc)

3 Structure generation module

test

3.1 test

daf

3.2 Building simple structures

test

3.3 Force field optimization

test

3.4 Custom geometries

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3.5 Chelating ligands

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3.6 Building custom structures

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5.1 Input file generation

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5.2 Jobscript generation

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6.1 Similarity search

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6.2 Database screening

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7.3 Wavefunction

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7.4 Cubefiles

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7.5 Molecular orbitals

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7.6 Natural Bonding Orbitals

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7.7 Delocalization indices

test

8 Extras

8.1 Updating the database

8.2 Jobscript generation

9 Command line options

Keyword	*Description*	*Default value*
General parameters		
-help	show help message	-
-i	input file	-
-rundir	directory for jobs	/home/user/Runs
-suff	suffix for jobs folder	-
-genall	generate complex both with and without FF opt.	False
Structure generation parameters		
-core	core structure	-
-ccatoms	custom core connection atom(s) indices	-
-replig	flag for modify/replace feature	False
-geometry	coordination geometry	oct (octahedral)
-coord	coordination number	6
-lig	ligand structure name, SMILES or file path	-
-ligocc	frequency of corresponding ligands	1
-keepHs	do not remove Hydrogens from ligand	False
-smicat	custom ligand connection atom(s) indices	-
-sminame	custom ligand name	-
-ligloc	force location of ligands on the template	False
-ligalign	smart alignment of ligands	True
-MLbonds	custom M-L bond length for ligand (A)	database value
-rgen	number of random generated molecules	1
-lignum	number of different ligands in random generation	-
-liggrp	ligand group for random generation	all
-ligctg	ligand category for random generation	all
-rkHs	keep Hydrogens for random generation	False
-ff	select force field for FF optimization	MMFF94
-ffoption	select when to perform FF optimization	Before & After
-distort	randomly distort backbone by x%	0%
-langles	custom angles (polar, azimuthal) for ligand	0/0

Extra molecules parameters		
-bind	extra molecule name, SMILES or file	False
-bcharge	binding species charge	0
-bph	azimuthal angle phi for binding species	random
-bref	reference atoms for placement of extra molecules	COM
-bsep	flag for separating extra molecule in input or xyz file	False
-btheta	polar angle theta for binding species	random
-place	azimuthal angle for binding species relative to core	random
-bindnum	number of binding species copies for random placement	1
-nambsmi	name of custom extra molecule	-
-maxd	maximum distance for molecule placement (A)	0.0
-mind	minimum distance for molecule placement (A)	0.0
-oxstate	oxidation state of the metal	0

Quantum chemistry input		
-qccode	quantum chemistry code	TeraChem
-charge	charge for system	0
-calccharge	flag to calculate charge	False
-spin	spin multiplicity for system	1
-runtyp	run type	optimize
-method	electronic structure method	ub3lyp
-basis	basis for terachem or qchem job	lacvp*
-dispersion	dispersion forces	False
-qoption	extra arguments for TeraChem in syntax	-
-exchange	exchange in qchem job	b3lyp
-correlation	correlation in qchem job	none
-remoption	extra arguments for qchem $rem block	-
-unrestricted	unrestricted calculation	True
-gbasis	GBASIS option in GAMESS	6
-ngauss	NGAUSS option in GAMESS	N31
-npfunc	NPFUNC option for diffuse functions in GAMESS	-
-ndfunc	NDFUNC option for diffuse functions in GAMESS	-
-sysoption	extra arguments for $SYSTEM GAMESS block	-
-ctrloption	extra arguments for $CONTRL GAMESS block	-
-scfoption	extra arguments for $SCF GAMESS block	-
-statoption	extra arguments for $STATPT GAMESS block	-

Jobscript parameters		
-jsched	job scheduling system	SGE
-jname	jobs main identifier	-
-memory	memory reserved per thread for job file in G	2G
-wtime	wall time requested in hours for queueing system	168h
-queue	queue name	gpus
-gpus	number of GPUS	1
-cpus	number of CPUs	1
-modules	modules to be loaded for the calculation	-
-joption	additional options for jobscript	-
-jcommand	additional commands for jobscript	-

Database search input		
-dbsim	SMILES/ligand/file for similarity search	-
-dbcatoms	connection atoms for similarity search	-
-dbresults	how many results for similary search or screening	-
-dboutputf	output file for search results	simres.smi
-dbbase	database for search	-
-dbsmarts	SMARTS string for screening	-
-dbfinger	fingerprint for similarity search	-
-dbatoms	number of atoms to be used in screening	-
-dbbonds	number of bonds to be used in screening	-
-dbarbonds	number of aromatic bonds to be used in screening	-
-dbsbonds	number of single bonds to be used in screening	-
-dbmw	molecular weight to be used in screening	-

Post-processing parameters		
-postp	post process results	-
-postqc	quantum chemistry code used	TeraChem
-postdir	directory with results	/home/user/Runs
-pres	generate calculations summary	False
-pdeninfo	calculate average properties for electron density	False
-pcharge	calculate charges	False
-pgencubes	generate cubefiles	False
-pwfninfo	get information about wavefunction	False
-pdeloc	get delocalization and localization indices	False
-porbinfo	get information about MO	False
-pnbo	post process nbo analysis	False