Jammy Key for Configurational Sampling

SCRIPT NAME	ARGUMENTS	DESCRIPTION	DEFAULT
	A SA	**ammonia + sulphuric acid**	default = A SA
JKCS0_copy	-all	(A,SA,GD,W,H,DMA,TMA,Ar)	
	-lm 1000	**save 1000 local minima in ABC**	default = 5000
	-gen 100	**100 generations in ABC**	default = 100
	-init 1000	**1000 initial structures in ABC**	default = 5000
JKCS1_prepare	**-sc 4**	**4 scout bees in ABC**	default = 4
JKCS2_runABC			
JKCS3_runXTB	-sp	just SP calc. … no optimization	
	-gibbs	**collect also Gibbs energies**	default = 10:00:00
JKCS4_collect	**[*folder*]**	**analyzed folder**	default = XTB
	[*file*]	**e.g.: resultsXTB.dat**	
	-rg 10	**filter out str. with Rg>10 A**	
	-d 15	**filter out str. with E>15 kcal/mol**	
	-dm 4	**-d 4*M, where M=# of molecules**	
	-s 100	**uniformly sample 100 str.**	
JKCS7_filter	-c3 4	perform 3D filtering: +column 4	
	-f [*folder*]	name of new folder	default = DFT
	-r [*NAME*]	data from resultsNAME.dat	default = XTB
	-m "# wb97xd opt"	method	default = "# wb97xd 6-31+g* opt"
JKCS5_runDFT	-p "DLPNO"	program (G16,XTB,DLPNO ..)	default = G16
sbatch JKsend JKCS6_commands	-m [*mailaddress*]	mail to sb in job end	

ADITIONAL ARGUMENTS FOR ALL JKCS SCRIPTS			
	-help	print help	
	-time	queuing time (10:00:00)	default = 72:00:00
	-par	partition (test, longrun)	default = serial
	-programs	2	default = programs.txt

QUEUEING			
sbatch JKrun	**[file(s).com]**	file to G16 (*file.log cannot exist*)	default = `ls *.com`
sbatch JKsend	**[script.sh or command]**	*e.g.*: echo 'Hi' *or* JKCS1_prepare	
GAUSSIAN			
	[file(s).xyz]	xyz file to be converted	default = `ls *.xyz`
	-method "[*method*]"	*e.g.*: "# HF 6-31+g* opt"	
JKxyz2com	**-char +1**	charge	default = 0
JKlog2com	**[file(s).log]**	log file(s) to be converted	default = `ls *.log`
	[file(s).log]	log file(s) to be converted	default = `ls *.log`
JKlog2xyz	-abc	create input for ABCluster	
	[file(s).log]	log file(s) to be analyzed	default = `ls *.log`
	-el	print electronic energy	
	-g	print Gibbs free energy	
	-d	print dipole moment	
JKgaussstat	-pol	print polarizability	
XTB			
JKxtb	-opt "-opt char +1"	options of GNF-*x*TB	