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The Distortion/Interaction Activation Strain (DIAS) analysis is a powerful tool for the investigation of energy barriers. However, setup and data analysis of such a calculation can be cumbersome and requires lengthy intervention of the user. We present autoDIAS, a python tool for the automated setup, performance, and data extraction of the DIAS analysis, including automated detection of fragments and relevant geometric parameters.

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autoDIAS: a python tool for an automated Distortion/Interaction Activation Strain Analysis

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ABSTRACT

The Distortion/Interaction Activation Strain (DIAS) analysis is a powerful tool for the investigation of energy barriers. However, setup and data analysis of such a calculation can be cumbersome and requires lengthy intervention of the user. We present autoDIAS, a python tool for the automated setup, performance, and data extraction of the DIAS analysis, including automated detection of fragments and relevant geometric parameters.

Introduction

The Distortion Interaction Analysis,¹ also known as Activation Strain Model (ASM),^{2,3} is an energy decomposition method which allows for chemically intuitive analysis of energy barriers.⁴ In the Distortion/Interaction Activation Strain (DIAS) analysis, which is a further development of energy decompositions introduced by Morokuma,⁵ the electronic energy ΔE of a complex, for example a transition state geometry, is dissected into two contributing factors.

$$\Delta E = \Delta E_{\text{dist}} + \Delta E_{\text{int}} \quad (1)$$

The distortion energy ΔE_{dist} (called strain energy ΔE_{strain} in the Activation Strain Model) describes the energy needed to distort the isolated fragments from their relaxed geometries to the geometry found in the complex. The interaction energy ΔE_{int} describes the usually stabilizing interaction between the fragments if they are brought together into the complex. This analysis can be applied to single geometries or multiple geometries along a scan or reaction coordinate, to provide information on the nature of interaction between the fragments and the potential energy surface. This method has been widely applied for a broad range of chemical systems such as cycloadditions,⁶⁻¹⁸ ene reactions,¹⁹ metal complexes and catalysis,²⁰⁻²⁷ organocatalysis,²⁸⁻³¹ and addition³² and substitution reactions.³³⁻³⁵

The implementation of a DIAS analysis is straight forward and can be performed using any electronic

structure software. It requires the calculation of the electronic energies of the relaxed fragments, the complex and the distorted fragments. The distortion energy for each fragment can then be calculated by subtracting the energy of the relaxed geometry while the interaction energy is the difference between the sum of distortion energies and the energy of the complex (Figure 1).

Figure 1. Calculations performed during a Distortion/Interaction Activation Strain analysis.

While this is, in theory, simple to realize it requires a large amount of effort in the preparation of the input files for the separated distorted fragments and the analysis regarding geometric parameters and energies. In addition, it has been shown that performing a DIAS analysis along a reaction or scan coordinate, rather than on a single point like a transition state, can be beneficial.^{36,37} However, this

requires the preparation and analysis of potentially large amounts of structures. Automation of these processes is needed for simple and efficient access to such DIAS analyses. To the best of our knowledge only few software packages aim to solve this problem; however, they are limited in functionality or to a certain electronic structure program. PyFrag,³⁸ the python tool that inspired autoDIAS, is a wrapper for the Amsterdam Density Functional (ADF, SCM, the Netherlands)^{39,40} software package. It allows for performance of a semi-automated Distortion/Interaction Activation Strain analysis, in this case called Activation Strain Model, and additional energy decomposition methods provided within ADF. While an excellent tool for the use with ADF it is limited to this electronic structure program. Recently Laloo *et al.* published an extension to the ExcelAutomat⁴¹ that aims for preparation of input files and plotting of the resulting data.⁴² While this makes good progress towards automation of the process, it does not provide a fully automated integration of a DIAS analysis and is limited in features.

In addition, autoDIAS includes several useful utilities, features and modes, including a reduction of the amount of calculated points in multi geometry DIAS calculations, a reordering of structures from IRC

calculations to present a continuous progress along the reaction coordinate, an automated detection of fragments, and an automated detection of forming/breaking bonds for multi geometry calculations.

Examples

In the following three examples of DIAS analyses are presented which were prepared using autoDIAS on the Hoffman2 cluster at UCLA. Gaussian 09 was used to prepare the input structures and as driver for the required single point energy calculations.

Reaction 1

The DIAS analysis was conducted on the transition state geometry of the cycloaddition between a tertiary azide and the strained cyclooctyne (1R,8S,9s)-Bicyclo[6.1.0]non-4-yn-9-ylmethanol (BCN) taken from a recent study about the reactivity of tertiary azides in strain-promoted alkyne-azide cycloadditions (Figure 3).⁷ Calculations were performed at the B3LYP/6-31G(d) level of theory. Fragments were automatically and correctly identified by autoDIAS. Input and structures were parsed in 35 ms, the required three Gaussian input files were prepared in 18 ms. The electronic energy of the transition state in relation to isolated reactants is 9.7 kcal/mol. ΔE_{int} is stabilizing with a value of -6.7 kcal/mol and ΔE_{dist} is destabilizing with a total value of 16.4 kcal/mol. The tertiary azide contributes mainly to this distortion energy with 14.7 kcal/mol while the distortion energy for BCN is only 1.7 kcal/mol.

Figure 3. DIAS analysis of the transition state between BCN and *tert*-butylazide. Energies in kcal/mol.

Figure 2. Workflow of autoDIAS.

Scan 1

A scan with 100 steps along the B-N distance in the trimethylamine-borane complex from 1.65 to 3.65 Å was performed in G09 at the M06-2X/6-31G(d) level of theory resulting in 101 structures. The Gaussian output file was used as input for autoDIAS. The structure parser method for scans and IRC calculations from G09 files implemented in autoDIAS does only extract converged structures. 81 converged structures were extracted, 20 non-converged structures were ignored. Automated Distortion/Interaction Activation Strain analysis was performed and is shown in Figure 4. Fragments and the relevant B-N bond was automatically detected by autoDIAS. Input and geometries were fetched in 23 seconds 309 ms, G09 input files for 81 structures (243 files) were prepared in 1 second 119 ms. Total energy, total distortion energy and interaction energy is plotted against the B-N distance. Note the missing points especially around 3 Å resulting from non-converged structures. This analysis shows that stabilizing interactions occur much earlier when moving the Lewis acid/base pair together, starting at a distance over 4 Å while distortion energies do not contribute significantly down to a distance of 2.5 Å.

Figure 4. DIAS analysis for a scan along the BN bond distance of the trimethylamine-borane complex. Energy in kcal/mol, distance in Å.

IRC 1

An IRC calculation of the archetypal Diels-Alder reaction between acrolein and 1,3-butadiene was performed in G09 at the M06-2X/6-31G(d) level of theory. The calculation resulted in 589 points along the IRC of which 90 were used for the DIAS analysis using the reduce option (RMSD threshold = 0.025) implemented in autoDIAS. The input file and structures were imported within 2 seconds and 651 ms, Gaussian input files for 90 structures were prepared in 762 ms. Fragments and both forming bonds were automatically and correctly detected. Total energy, distortion energies of both fragments, total distortion energy and interaction action are plotted against the shorter forming bond (Figure 5).

Figure 5. DIAS analysis of the Diels-Alder reaction between acrolein and 1,3-butadiene. Transition state geometry shown on the right. Energy in kcal/mol, distance in Å.

Technical Details

autoDIAS was written in Python for use under Linux. It can therefore be used on most local machines and HPC clusters. A version for Windows 10 was not prepared since the availability of the Ubuntu subsystem under Windows (WSL) allows running Linux software natively on Windows computers. autoDIAS is compatible and was tested with Python versions 2.6 and higher, however, we recommend the use of Python 3.5 or higher. autoDIAS was tested on the Windows 10 Ubuntu subsystem on a personal computer, on the Hoffman2 cluster at UCLA and the Vienna Scientific Cluster 3 (VSC3, Vienna, Austria). The most up-to-date version is available for download on GitHub. Gaussian 09 Revision D.01,⁴⁴ Gaussian 16 Revision A.03,⁴⁵ ORCA 4.0.1.2,⁴⁶ Q-Chem 4.3⁴⁷ and NWChem 6.6⁴⁸ were used as drivers. Chemcraft 1.8 was used for visualization.⁴⁹

To use autoDIAS one must provide two input files; 1) A file containing molecular geometries, at the moment single or multi structure XYZ files or Gaussian output files and 2) an input file containing the needed information to perform the DIAS analysis. This includes the name of the file containing the structures, details about the structures and fragments, such as charge and multiplicity, information about the analysis such as what bonds, angles or dihedral angles should be extracted, information about further settings such as which files to keep after the analysis and information about how calculations using the selected driver are performed. The last section allows for easy adaption of other

computational chemistry software packages and the use on different systems with different commands for running these calculations. An example of an input file with detailed descriptions of the settings can be found in the supporting information and is included in the software package.

autoDIAS accepts XYZ files and Gaussian output files as input. Possible Gaussian files include output from single point, frequency analysis, geometry optimizations, combined geometry optimization frequency analysis, IRC and scan jobs. In case of IRC and scan jobs only converged points are extracted. This can be circumvented by converting the output file in a XYZ file containing all structures and using this as input for autoDIAS, however, using non-converged structures is not advised. Figure 6 shows the extracted (black) and omitted (red) points for **scan 1**.

Figure 6. Visualization of the omitted, non-converged points (red) for the electronic energy of **scan 1**. Energy in kcal/mol, distances in Å.

IRC calculations in Gaussian which are performed in both directions start at the provided transition state geometry and are first propagated in one direction and then propagated in the other direction starting from the transition state again. However, this means that extracted geometries do not represent a continuous progress along the reaction coordinate. The **reorder** setting provides a tool that corrects this error but can potentially be used in any cases in which two continuous series of geometries are stitched together in an incorrect orientation. This is realized by calculating the RMSD, using the Procrustes analysis on centroid centered structures, between any two consecutive structures. If at least one of the RMSDs between two geometries is more

than three times the average RMSD the point with the biggest RMSD is detected as the cut between the two separate parts. RMSD calculations are then performed between the first and last points of each part and orders within the parts are reversed to minimize the structural difference at the cut (Figure 7).

Figure 7. Reordering of the points in **IRC 1**. Energy in kcal/mol. The dashed line in the RMSD plot represents the threshold of 3 times the average RMSD.

From the provided input structures, fragments are produced by slicing the geometries according to provided lists of atom numbers in each fragment. Since providing such lists can be cumbersome, especially for larger molecules, autoDIAS provides two utilities to reduce the needed input. The first method requires the input of the atom list for one fragment, the atom list for the other fragment is then automatically determined. The second method is the completely automated determination of two fragments by providing no input in this regard. Fragment 1 will be the one including the first atom in the structure, which is helpful for naming fragments and providing relaxed geometry energies for calculation of distortion and relative energies. The automatic fragment detection will fail if only structures with lower fragment numbers than 2 are provided. If more than two fragments are detected some will be combined to result in two fragments. Fragments are determined by connecting atoms through bonds and grouping continuously connected

atoms. Bonds are defined by using covalent radii⁵⁰ for each atom type plus a 25% overhead. In case of an analysis of multiple structures where it might occur that two fragments become one over the progress of the analyzed coordinate the two fragments that occur most often are chosen.

Calculations containing a big amount of structures can be computationally expensive. The **reduce** option allows for a reduction of overall number of structures to reduce the calculation time. This utility is inspired by a similar tool used in the Bickelhaupt group in combination with PyFrag. Starting by selecting the first point, consecutive points are deleted if the RMSD between that structure and the currently selected one is below a provided threshold. Once a structure is reached that differs by more than threshold this structure is selected, and the progress is repeated until the last structure is reached. Figure 8 shows the effect of this reduction on the electronic energy of the analysis of an IRC calculation using G09 of Diels-Alder reaction **IRC 1**. This calculation was performed using the IRC=(stepsize=1) setting in G09 to produce a large amount of points along the IRC, resulting in 589 points. Using reduce in combination with a RMSD threshold of 0.005 Å reduces the amount of points by 71.5%. Using 0.01 Å as threshold the amount is reduced by another 13.2% down to 15.3% of total points. A threshold of 0.025 Å reduces the amount to only 39 points (6.6%) while still providing a good image of the energy progress along the reaction coordinate.

Figure 8. Comparison between the result using different levels of the reduce utility in autoDIAS for **IRC 1**. Electronic energy in kcal/mol is shown.

Analysis of the performed calculation can be requested by using the analysis keyword (Analysis = YES). Not using this option is necessary in case of a driver or performed calculation for which no parser for the energy is implemented in autoDIAS. Extraction of geometric parameters is important for multi structure DIAs, allowing for analysis and plotting along selected coordinates. autoDIAS allows for extraction of bond lengths, angles and dihedral angles. Parameters which should be extracted can be specified in the input file. autoDIAS allows for **automatic detection of bonds**. This is requested by using the keyword “auto” in the geometry bond section of the input file, providing no input in this section or providing only incorrect input. This automated process does only work correctly in case of multiple geometry calculations and is performed by calculating the changes in bond orders, determined as described for the automated fragment detection. The two bonds that change the fewest times but at least once over the progress of the scan/reaction coordinate are selected. This crude method provided good results in all tested cases. Bonds were automatically and correctly detected in all presented cases. Bond angles are requested by providing 3 atoms in the angle input section and dihedral angles are requested by specifying 4 atoms. Invalid requests are ignored.

Several further settings are available. These include the option to delete keep all calculation input files (Keep input files = YES), produce XYZ files for all structures, fragments, and a file including all structures in one file (Keep xyz = YES), and keep the log file providing information about the performed DIAS analysis (Keep log file = YES).

In addition, the **prepare only** mode requests reading of the input file and preparation of the input and *.xyz files. If necessary automatic detection of fragments, reduction of structures, and reordering is also performed. This mode allows for determination if the automated fragment and bond detection works correctly or if the chosen RMSD threshold for the reduce option reduces the number of calculated

points to a reasonable amount. It can also be used to prepare the needed input file before running the needed calculations on a different system and/or in parallel.

The **analysis only** mode requests analysis of the previously generated output files only. This can be useful to add further geometric parameters to the analysis or add previously missing fragment energies. It can be requested using the “-a” flag. This mode ignores all input regarding the execution of the prepared input files and prepares an DIA analysis file equal to that produced during normal autoDIAS operation. It is to note that this modus still parses the structure input file and performs any requested changes (i.e. reduction of points and reordering) to fetch geometry data.

The user needs to provide a template for the input for the single point calculation for the chosen driver in the layout section. Wildcards can be used for filename, charge, multiplicity and (cartesian) coordinates. In addition, the user has to provide the file extensions for input and output files for these calculations, and the syntax for performing the calculation on the given computer system in the run_job section of the input file, using Wildcards for input and output file names.

Minimal input for an analysis using autoDIAS are the file name of the file containing the structures, charges and multiplicities and information about running the calculations (layout and run_job sections). In addition, input of fragment energies is advised.

Output is provided in a text-based file named <jobname>_DIAS.txt listing all requested geometric parameters and calculated energies. The numpy “genfromtxt” and the MS Excel “text to columns” functions can be used to convert the data into an array that can be used for further manipulation or plotting. An additional log file is provided named <jobname>_log.txt containing information about the analysis and timing, this file is deleted after successful completion in case the keep log option is set to NO. Input and output files from energy calculations and xyz files are produced/kept if the corresponding options are set.

Performance

Performance of autoDIAS was investigated using the Windows 10 Ubuntu subsystem and Python 3.7.1 on a Dell XPS13 9370 equipped with an Intel i7-8550u CPU and 16GB of memory. Several operations within autoDIAS could be optimized for speed. However, performance examples shown in Table 1 demonstrate that operations even for hundreds of structures only take some seconds. Reordering of structures adds approx. 10% time to the time spend in producing input structures. The time for parsing the structures which includes splitting them into

fragments and reading the input file strongly depends on the nature and size of the input file while the time for producing the input files and performing analysis depends on the amount of structures. On average 120 ± 40 input files were produced per second and 760 ± 170 files were analyzed per second. Compared to the amount of time needed to perform energy calculations time spend in input file parsing, input file creation and analysis is neglectable.

Figure 8. Performance demonstration.

	File size	File type	Converged structures	Reorder	Reduce	Resulting points	Used driver	Time for parsing [s]	Time for producing input files [s]	Time for analysis [s]
Scan 1	66 MB	G09 (scan)	81	No	No	81	G09	5.071	1.756	0.282
	84 KB	XYZ (multi)	101	No	No	101		0.137	2.216	0.324
IRC 1	5.5 MB	G09 (IRC)	589	Yes	No	589		0.935	12.488	3.215
				No	No	589		0.945	11.499	3.222
				Yes	Yes (0.005)	168		0.936	3.277	0.607
				Yes	Yes (0.01)	90		0.973	1.786	0.330
				No	Yes (0.01)	90		0.974	1.582	0.313
				Yes	Yes (0.025)	39		0.983	0.806	0.103
								0.020	0.054	0.004
Reaction 1	60 KB	G09 (SP)	1	No	No	1		0.060	0.035	0.005
	605 KB	G09 (Opt)	1	No	No	1		0.018	0.036	0.004
	332 KB	G09 (Freq)	1	No	No	1		0.060	0.040	0.004
	977 KB	G09 (Opt Freq)	1	No	No	1		0.010	0.038	0.005
	3 KB	XYZ (single)	1	No	No	1	ORCA	0.011	0.035	0.005
							NWChem	0.013	0.038	0.003
							Q-Chem			

Conclusions

We present autoDIAS, a python tool for the automated Distortion/Interaction Activation Strain analysis. This tool allows for the automated setup, performance and analysis of a DIAS analysis, even for big amount of structures. autoDIAS is easy to use, high performing, requires little input, can be used with many electronic structure programs and even allows for a Distortion/Interaction

Activation Strain analysis along a two, or more, dimensional potential energy surface. We are confident that autoDIAS will be a useful tool for computational chemists who wish to analyze energy barriers and surfaces using the Distortion/Interaction Activation Strain analysis.

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Keywords: Computational chemistry, Bond theory, Distortion, Strain, Software

((Additional Supporting Information may be found in the online version of this article.))

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GRAPHICAL ABSTRACT

Dennis Svatoněk and Kendall N. Houk

autoDIAS: a python tool for an automated Distortion/Interaction Activation Strain Analysis

Performing a Distortion/Interaction Activation Strain analysis can be cumbersome due to the potentially large amount of needed calculations which have to be prepared, run, and analyzed. autoDIAS is a python tool that helps automating this process while including a range of useful additional tools.

autoDIAS.pdf (682.74 KiB)

[view on ChemRxiv](#) • [download file](#)

autoDIAS

Automated Distortion/Interaction Activation Strain Analysis

autoDIAS.png (64.09 KiB)

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Supporting Information

autoDIAS: a python tool for an automated Distortion/Interaction Activation Strain Analysis

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autoDIAS

An up to date version of autoDIAS can be found on GitHub:

<https://github.com/dsvatunek/autoDIAS>

The autoDIA Stool consists of 4 python files:

autoDIAS.py	controls the analysis, produces input files for drivers, produces the log file
DIAS_inputparser	parses settings and structures, checks input for wrong information, does the automated fragment and bond detection and prepares the fragment structures
DIAS_reduce_reorder	responsible for the reduce and reorder functions of autoDIAS
DIAS_analysis	parses energies and geometric parameters, plots the result to the DIAS file

autoDIAS.py

```
#!/usr/bin/env python
banner="""
*****
*****

                                autoDIAS
                                Dennis Svatunek
                                UCLA
                                d.svatunek@chem.ucla.com
                                @clickchemist

                                Download the newest version from:
                                https://github.com/dsvatunek/autoDIAS

                                Please cite. DOI: 10.26434/chemrxiv.7789940
*****
*****

Python wrapper for several computational chemistry software packages to
automatically
perform a Distortion/Interaction Activation Strain analysis calculations.

*****
*****
"""
from DIAS_inputparser import *
from DIAS_analysis import *
from DIAS_reduce_reorder import *
import argparse, sys, time, subprocess, os, datetime, copy
__version__ = '1.0.0'
__author__ = 'Dennis Svatunek'
__email__ = "d.svatunek@chem.ucla.edu"
try:
    range = xrange
except NameError:
    pass
def save_xyz(A, atoms, title, filename):
    file = open(filename + '.xyz', 'w')
    file.write(str(len(atoms))+ "\n"+ title + "\n")
    for i in range(len(A)):
        file.write("{0:2s} {1:15.12f} {2:15.12f}
{3:15.12f}\n".format(atoms[i], A[i, 0], A[i, 1], A[i, 2]))
    file.close()
    return
def save_input(A, atoms, title, filename, jobname, g09structure, charge,
multiplicity):
    file = open(filename, 'w')
    coordinates = ""
    for i in range(len(A)):
        coordinates = coordinates +("{0:2s} {1:15.12f} {2:15.12f}
{3:15.12f}\n".format(atoms[i], A[i, 0], A[i, 1], A[i, 2]))
    g09structure = g09structure.replace("$multiplicity", str(multiplicity))
    g09structure = g09structure.replace("$charge", str(charge))
    g09structure = g09structure.replace("$filename", jobname)
    g09structure = g09structure.replace("$coordinates", coordinates.strip())
    file.write(g09structure)
```

```

file.close()
return
def molecular_formula(atoms):
    alphabetic_periodic_table = sorted(copy.deepcopy(periodic_table))
    formula = ""
    count = []
    for element in alphabetic_periodic_table:
        if count[alphabetic_periodic_table.index("C")] > 1:
            formula = formula + 'C' +
str(count[alphabetic_periodic_table.index("C")])
            count[alphabetic_periodic_table.index("C")] = 0
        elif count[alphabetic_periodic_table.index("C")] > 0:
            formula = formula + 'C'
            count[alphabetic_periodic_table.index("C")] = 0

        if count[alphabetic_periodic_table.index("H")] > 1:
            formula = formula + 'H' +
str(count[alphabetic_periodic_table.index("H")])
            count[alphabetic_periodic_table.index("H")] = 0
        elif count[alphabetic_periodic_table.index("H")] > 0:
            formula = formula + 'H'
            count[alphabetic_periodic_table.index("H")] = 0

    for x in range(0, len(alphabetic_periodic_table)):
        if count[x] == 1:
            formula = formula + alphabetic_periodic_table[x]
        elif count[x] > 1:
            formula = formula + alphabetic_periodic_table[x] + str(count[x])
    return formula
def main():
    parser = argparse.ArgumentParser(usage='% (prog)s inp_file')
    parser.add_argument('inp_file', metavar='Input file', type=str,
help='Name of the input file')
    parser.add_argument("-a", "--analysis", action='store_true',
help='Analysis only', default=False)
    if len(sys.argv) == 1:
        parser.print_help()
        sys.exit(1)
    args = parser.parse_args()
    overallstarttime=time.time()
    starttime=time.time()
    settings, structures = parse_in(args.inp_file,args.analysis)

    if args.analysis:
        endtime=time.time()
        totaltime=str(endtime-starttime)
        seconds=totaltime.split('.')[0]
        milliseconds=float('0.'+totaltime.split('.')[1])*1000
        print('Processed input and parsed structures in {0} seconds and
{1:.0f} ms'.format(seconds, float(milliseconds)))
        if settings.reorder:
            structures = reorder(structures)
        if settings.reduce:
            structures = reduce(structures, settings)
        analysis_only(structures,settings)
    return

```

```

endtime=time.time()
totaltime=str(endtime-starttime)
seconds=totaltime.split('.')[0]
milliseconds=float('0.'+totaltime.split('.')[1])*1000
log = open(settings.logfile, 'a')
log.write(banner)
try:
    hostname = subprocess.check_output(['hostname']).decode('utf-8')
    username = subprocess.check_output(['whoami']).decode('utf-8')
except AttributeError:
    hostname= ""
    username= ""
log.write(str(username).strip()+'@'+str(hostname).strip()+'\n')
log.write(time.ctime()+'\n')
log.write('-----\n')
log.write('Input file: '+args.inp_file)
log.write('\nProcessed input and parsed structures in {0} seconds and
{1:.0f} ms\n'.format(seconds, float(milliseconds)))
log.write('-----\n')
log.write('Determined settings and variables: \n\n')
log.write('{0:50}{1}\n'.format("Job name",settings.name))
log.write('{0:50}{1}\n'.format("Structure input",settings.ircfile))
log.write('{0:50}{1}\n'.format("Structure input
filetype",settings.filetype))
if settings.analysis:
    log.write('{0:50}{1}\n'.format("\nAnalysis will be performed","YES"))
    if len(settings.geo_dist) > 0:
        log.write('    {0:50}\n'.format("The following bond distances
will be examined:\n"))
        for i in range(len(settings.geo_dist)):
            log.write('        {0:15}atom 1: {1}\n        {2:15}atom 2:
{3}\n\n'.format("Bond
"+str(i+1),settings.geo_dist[i][0],"",settings.geo_dist[i][1]))
            if len(settings.geo_ang) > 0:
                log.write('    {0:50}\n'.format("The following angles will be
examined:\n"))
                for i in range(len(settings.geo_ang)):
                    log.write('        {0:15}atom 1: {1}\n        {2:15}atom 2:
{3}\n        {2:15}atom 3: {4}\n\n'.format("Angle
"+str(i+1),settings.geo_ang[i][0],"",settings.geo_ang[i][1],settings.geo_ang[
i][2]))
                    if len(settings.geo_dih) > 0:
                        log.write('    {0:50}\n'.format("The following dihedral angles
will be examined:\n"))
                        for i in range(len(settings.geo_dih)):
                            log.write('        {0:15}atom 1: {1}\n        {2:15}atom 2:
{3}\n        {2:15}atom 3: {4}\n        {2:15}atom 4:
{5}\n\n'.format("Dihedral
"+str(i+1),settings.geo_dih[i][0],"",settings.geo_dih[i][1],settings.geo_dih[
i][2],settings.geo_dih[i][3]))
                            log.write('{0:50}{1}\n'.format("Keep xyz files","YES" if settings.keepxyz
else "NO"))
                            log.write('{0:50}{1}\n'.format("Keep input files","YES" if
settings.keepinput else "NO"))
                            log.write('{0:50}{1}\n'.format("Keep output files","YES" if
settings.keepoutput else "NO"))

```

```

log.write('{0:50}{1}\n'.format("Keep this log file","YES" if
settings.keeplog else "NO"))
log.write('{0:50}{1}\n'.format("Reorder structures","YES" if
settings.reorder else "NO"))
log.write('{0:50}{1}\n'.format("Reduce structures","YES" if
settings.reduce else "NO"))
if settings.reduce:
    log.write('{0:50}{1}\n'.format("Threshold for reducing
structures",settings.reduce_tresh))
    log.write('{0:50}{1}\n'.format("Prepare input and exit","YES" if
settings.prepareonly else "NO"))
    formula = molecular_formula(structures.atoms)
    fragment1_formula = molecular_formula(structures.frag1atoms)
    fragment2_formula = molecular_formula(structures.frag2atoms)
    log.write('\nStructure information\n\n')
    log.write('Input structure has {0} atoms with a molecular formula
of:{1:>15}\n\n'.format(len(structures.atoms), formula))
    log.write('{0} has {1} atoms with a molecular formula
of:{2:>15}\n\n'.format(settings.frag1name, len(structures.frag1atoms),
fragment1_formula))
    log.write('{0} has {1} atoms with a molecular formula
of:{2:>15}\n\n'.format(settings.frag2name, len(structures.frag2atoms),
fragment2_formula))
    log.write('Complex has a charge and multiplicity of: {0}
{1}\n'.format(settings.charge, settings.multi))
    log.write('{0} has a charge and multiplicity of: {1}
{2}\n'.format(settings.frag1name, settings.frag1charge, settings.frag1multi))
    log.write('{0} has a charge and multiplicity of: {1}
{2}\n'.format(settings.frag2name, settings.frag2charge, settings.frag2multi))
    log.write('{0} has an energy of: {1}\n'.format(settings.frag1name,
settings.frag1energy))
    log.write('{0} has an energy of: {1}\n'.format(settings.frag2name,
settings.frag2energy))
    log.write('\n')
    log.write('-----\n')
    log.close()
if settings.reorder:
    structures = reorder(structures)
if settings.reduce:
    structures = reduce(structures, settings)
starttime=time.time()
if settings.keepxyz:
    if not os.path.exists(settings.name+'_xyz'):
        os.makedirs(settings.name+'_xyz')
    for x in range(0, len(structures.xyz)):
        save_xyz(structures.xyz[x], structures.atoms,
structures.title[x], settings.name+'_xyz/complex_{0:04d}'.format(x+1))
        save_xyz(structures.xyz_1[x],
structures.frag1atoms,settings.frag1name+'__{0:04d}'.format(x+1),
settings.name+'_xyz/'+settings.frag1name+'__{0:04d}'.format(x+1))
        save_xyz(structures.xyz_2[x],
structures.frag2atoms,settings.frag2name+'__{0:04d}'.format(x+1),
settings.name+'_xyz/'+settings.frag2name+'__{0:04d}'.format(x+1))
        os.system("cat {0}_xyz/complex*.xyz >
{0}_xyz/complete.xyz".format(settings.name))
    if not os.path.exists(settings.name+'_input'):
        os.makedirs(settings.name+'_input')

```

```

if not os.path.exists(settings.name+'_output'):
    os.makedirs(settings.name+'_output')

for x in range (0, len(structures.xyz)):
    save_input(structures.xyz[x], structures.atoms, structures.title[x],
settings.name+'_input/complex_{0:04d}'.format(x+1)+settings.input_file_exten
sion, settings.name+'_output/complex_{0:04d}'.format(x+1),
settings.inputlayout, settings.charge, settings.multi)
    save_input(structures.xyz_1[x], structures.fraglatoms,
settings.fraglname+'__{0:04d}'.format(x+1),
settings.name+'_input/'+settings.fraglname+'__{0:04d}'.format(x+1)+settings.i
nput_file_extension,
settings.name+'_output/'+settings.fraglname+'__{0:04d}'.format(x+1),
settings.inputlayout, settings.fraglcharge, settings.fraglmulti)
    save_input(structures.xyz_2[x], structures.frag2atoms,
settings.frag2name+'__{0:04d}'.format(x+1),
settings.name+'_input/'+settings.frag2name+'__{0:04d}'.format(x+1)+settings.i
nput_file_extension,
settings.name+'_output/'+settings.frag2name+'__{0:04d}'.format(x+1),
settings.inputlayout, settings.frag2charge, settings.frag2multi)
    endtime=time.time()
    totaltime=str(endtime-starttime)
    seconds=totaltime.split('.')[0]
    milliseconds=float('0.'+totaltime.split('.')[1])*1000
    log = open(settings.logfile, 'a')
    log.write('Produced input files for {0} structures in {1} seconds and
{2:.0f} ms\n'.format(len(structures.xyz),seconds, float(milliseconds)))
    log.write('-----\n')
    log.close()
    if settings.analysis and not settings.prepareonly:
        create_analysis_file(settings)
        log = open(settings.logfile, 'a')

    if settings.prepareonly:
        log.write('No calculations requested!\n')
    else:
        for x in range (0, len(structures.xyz)):

            command = settings.submit_setting.replace("$input",
settings.name+'_input/complex_{0:04d}'.format(x+1)+settings.input_file_exten
sion)
            command = command.replace("$output",
settings.name+'_output/complex_{0:04d}'.format(x+1)+settings.output_file_ext
ension)
            log.write(time.ctime()+'{0:<30}'.format('\tStarting
{0:>15}'.format('complex_{0:04d}'.format(x+1))))
            log.flush()
            starttime=time.time()
            os.system(command)
            endtime=time.time()
            totaltime=endtime-starttime
            log.write('\t finished after
{0:0>15}\n'.format(str(datetime.timedelta(seconds=totaltime))))
            log.flush()

```

```

        command = settings.submit_setting.replace("$input",
settings.name+'_input/'+settings.frag1name+'_{0:04d}'.format(x+1)+settings.i
nput_file_extension)
        command = command.replace("$output",
settings.name+'_output/'+settings.frag1name+'_{0:04d}'.format(x+1)+settings.
output_file_extension)
        log.write(time.ctime()+'{0:<30}'.format('\tStarting
{0:>15}'.format(settings.frag1name+'_{0:04d}'.format(x+1))))
        log.flush()
        starttime=time.time()
        os.system(command)
        endtime=time.time()
        totaltime=endtime-starttime
        log.write('\t finished after
{0:0>15}\n'.format(str(datetime.timedelta(seconds=totaltime))))
        log.flush()

        command = settings.submit_setting.replace("$input",
settings.name+'_input/'+settings.frag2name+'_{0:04d}'.format(x+1)+settings.i
nput_file_extension)
        command = command.replace("$output",
settings.name+'_output/'+settings.frag2name+'_{0:04d}'.format(x+1)+settings.
output_file_extension)
        log.write(time.ctime()+'{0:<30}'.format('\tStarting
{0:>15}'.format(settings.frag2name+'_{0:04d}'.format(x+1))))
        log.flush()
        starttime=time.time()
        os.system(command)
        endtime=time.time()
        totaltime=endtime-starttime
        log.write('\t finished after
{0:0>15}\n'.format(str(datetime.timedelta(seconds=totaltime))))
        log.flush()
        if settings.analysis:
            analysis(settings, structures, x)
            totaltime=time.time()-overallstarttime
            log.write('-----\n')
            log.write(time.ctime()+'\t Finished after
{0:0>15}\n'.format(str(datetime.timedelta(seconds=totaltime))))
            log.write('-----\n')
            log.close()
        if settings.keepinput == False:
            shutil.rmtree("input/", ignore_errors=True)
        if settings.keepoutput == False:
            shutil.rmtree("output/", ignore_errors=True)
        if settings.keeplog == False:
            os.remove(settings.logfile)

if __name__ == "__main__":
    main()

```


DIAS_inputparser

```
import numpy as np
import sys
import re
def line_prependers(filename, line):
    with open(filename, 'r+') as f:
        content = f.read()
        f.seek(0, 0)
        f.write(line.rstrip('\r\n') + '\n' + content)
class structures:
    pass
periodic_table =
["", "H", "He", "Li", "Be", "B", "C", "N", "O", "F", "Ne", "Na", "Mg", "Al", "Si", "P", "S", "
Cl", "Ar", "K", "Ca", "Sc", "Ti", "V", "Cr", "Mn", "Fe", "Co", "Ni", "Cu", "Zn", "Ga", "Ge",
"As", "Se", "Br", "Kr", "Rb", "Sr", "Y", "Zr",

"Nb", "Mo", "Tc", "Ru", "Rh", "Pd", "Ag", "Cd", "In", "Sn", "Sb", "Te", "I", "Xe", "Cs", "Ba
", "La", "Ce", "Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb", "Dy", "Ho", "Er", "Tm", "Yb", "Lu",
"Hf", "Ta", "W", "Re", "Os", "Ir", "Pt", "Au", "Hg", "Tl",

"Pb", "Bi", "Po", "At", "Rn", "Fr", "Ra", "Ac", "Th", "Pa", "U", "Np", "Pu", "Am", "Cm", "Bk
", "Cf", "Es", "Fm", "Md", "No", "Lr", "Rf", "Db", "Sg", "Bh", "Hs", "Mt", "Ds", "Rg", "Uub"
, "Uut", "Uuq", "Uup", "Uuh", "Uus", "Uuo"]
covalent_radii =
[0.00, 0.32, 0.28, 1.28, 0.96, 0.84, 0.76, 0.71, 0.66, 0.57, 0.58, 1.66, 1.41, 1.21, 1.11, 1
.07, 1.05, 1.02, 1.06, 2.03, 1.76, 1.70, 1.60, 1.53, 1.39, 1.61, 1.52, 1.50, 1.24, 1.32, 1.2
2, 1.22, 1.20, 1.19, 1.20, 1.20, 1.16, 2.20, 1.95, 1.90, 1.75,

1.64, 1.54, 1.47, 1.46, 1.42, 1.39, 1.45, 1.44, 1.42, 1.39, 1.39, 1.38, 1.39, 1.40, 2.44, 2.
15, 2.07, 2.04, 2.03, 2.01, 1.99, 1.98, 1.98, 1.96, 1.94, 1.92, 1.92, 1.89, 1.90, 1.87, 1.87
, 1.75, 1.70, 1.62, 1.51, 1.44, 1.41, 1.36, 1.36, 1.32, 1.45,

1.46, 1.48, 1.40, 1.50, 1.50, 2.60, 2.21, 2.15, 206, 2.00, 1.96, 1.90, 1.87, 180, 169, 1.80,
1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.80, 1.
80, 1.80, 1.80, 1.80, 1.80, 1.80]
def getDistance(atom1, atom2):
    distance = 0.00
    distance = np.sqrt((atom1[0]-atom2[0])**2+(atom1[1]-
atom2[1])**2+(atom1[2]-atom2[2])**2)
    return distance
def isInt(s):
    try:
        int(s)
        return True
    except ValueError:
        return False
def molecular_formula(atoms):
    alphabetic_periodic_table = sorted(copy.deepcopy(periodic_table))
    formula = ""
    count = []
    for element in alphabetic_periodic_table:
        count = count + [atoms.count(element)]
    if count[alphabetic_periodic_table.index("C")] > 1:
        formula = formula + 'C' +
str(count[alphabetic_periodic_table.index("C")])
        count[alphabetic_periodic_table.index("C")] = 0
```

```

elif count[alphabetic_periodic_table.index("C")] > 0:
    formula = formula + 'C'
    count[alphabetic_periodic_table.index("C")] = 0
if count[alphabetic_periodic_table.index("H")] > 1:
    formula = formula + 'H' +
str(count[alphabetic_periodic_table.index("H")])
    count[alphabetic_periodic_table.index("H")] = 0
elif count[alphabetic_periodic_table.index("H")] > 0:
    formula = formula + 'H'
    count[alphabetic_periodic_table.index("H")] = 0
for x in range(0, len(alphabetic_periodic_table)):
    if count[x] == 1:
        formula = formula + alphabetic_periodic_table[x]
    elif count[x] > 1:
        formula = formula + alphabetic_periodic_table[x] + str(count[x])
return formula
def isBond(distance, atomtype1, atomtype2, covalent_radii):
    bond = True
    '''find bond threshold based on covalent radii
    taken from 10.1039/b801115j
    For everything beyond Cm 1.80 A was used.
    get radii from saved numpy array
    use atomtypes as numbers
    use factor to be sure to catch bonds. Bigger factor means more bonds are
    detected
    '''
    atomtype1 = int(periodic_table.index(atomtype1))
    atomtype2 = int(periodic_table.index(atomtype2))
    bond_threshold = 1.25 *
(covalent_radii[atomtype1]+covalent_radii[atomtype2])
    if distance > bond_threshold:
        bond = False
    return bond
def getFragments(structure, atoms):
    adjacency_matrix = []
    for i in range(0, len(structure)):
        distances = []
        for j in range(0, len(structure)):
            distances = distances + [getDistance(structure[i], structure[j])]
        adjacency_matrix = adjacency_matrix + [distances]
    for i in range(0, len(adjacency_matrix)):
        for j in range(0, len(adjacency_matrix[i])):
            if isBond(adjacency_matrix[i][j], atoms[i], atoms[j],
covalent_radii):
                adjacency_matrix[i][j] = 1
            else:
                adjacency_matrix[i][j] = 0
    for i in range(0, len(adjacency_matrix)):
        adjacency_matrix[i] = [j+1 for j,x in enumerate(adjacency_matrix[i])
if x == 1]
    fragments = [adjacency_matrix[0]]
    for i in range (1, len(adjacency_matrix)):
        for j in range(0, len(fragments)):
            if len(set(adjacency_matrix[i]) & set(fragments[j])) > 0:
                fragments[j] = list(set(fragments[j]+adjacency_matrix[i]))
                break
        else:

```

```

        fragments = fragments + [adjacency_matrix[i]]
n_frag_old=len(fragments)
n_frag_new=-5
while n_frag_old != n_frag_new:
    n_frag_old=len(fragments)
    new_fragments = [sorted(fragments[0])]
    for i in range(0, len(fragments)):
        for j in range(0, len(new_fragments)):
            if len(set(fragments[i]) & set(new_fragments[j])) > 0:
                new_fragments[j] =
sorted(list(set(new_fragments[j]+fragments[i])))
                break
        else:
            new_fragments = new_fragments + [fragments[i]]
    fragments=new_fragments
    n_frag_new=len(fragments)
return fragments
def getConnectivity(structure):
    connectivity_matrix = np.zeros((len(structure),len(structure)))
    for i in range(0,len(connectivity_matrix )):
        for j in range(0,len(connectivity_matrix)):
            distance=getDistance(structure[i],structure[j])
            if isBond(distance,structures.atoms[i],
structures.atoms[j],covalent_radii):
                connectivity_matrix[i][j] = 1
            else:
                connectivity_matrix[i][j] = 0
    return connectivity_matrix
def getBonds(structures):
    count = np.zeros((structures.xyz[0].shape[0],structures.xyz[0].shape[0]))
    connectivity_old = getConnectivity(structures.xyz[0])
    for element in structures.xyz:
        connectivity = getConnectivity(element)
        for i in range(0, len(connectivity)):
            for j in range(0, len(connectivity[i])):
                if connectivity[i][j] != connectivity_old[i][j]:
                    count[i][j] = count[i][j] +1
        connectivity_old= connectivity
    for i in range(0,len(count)):
        for j in range(0, len(count)):
            if i >= j:
                count[i][j] = 0
    count[count == 0] = 1000
    freq = np.amin(count)
    geodist = [[int(np.where(count == freq)[0][0])+1,int(np.where(count ==
freq)[1][0])+1]]
    count[np.where(count == freq)[0][0],np.where(count == freq)[1][0]] = 1001
    freq = np.amin(count)
    geodist = geodist + [[int(np.where(count ==
freq)[0][0])+1,int(np.where(count == freq)[1][0])+1]]
    return geodist
def duplicates(int_list):
    int_list = sorted(int_list)
    duplicates = False
    for i in range (0, len(int_list)-1):
        if int_list[i] == int_list[i+1]:
            duplicates = True

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        else:
            pass
        return duplicates
def auto_frag(structures, settings):
    list_of_fragments = []
    for i in range(0, len(structures.xyz)):
        list_of_fragments = list_of_fragments +
[getFragments(structures.xyz[i], structures.atoms)]
    n_fragments = []
    for i in range(0, len(list_of_fragments)):
        n_fragments = n_fragments + [len(list_of_fragments[i])]
    twofrag = False
    morefrag = False
    for element in n_fragments:
        if element == 2:
            twofrag = True
            break
        if element > 2:
            morefrag = True
    if twofrag:
        indices = [i for i, x in enumerate(n_fragments) if x == 2]
        counts = [list_of_fragments.count(list_of_fragments[x]) for x in
indices]
        fragments = list_of_fragments[indices[counts.index(max(counts))]]
        settings.fraglatoms = np.sort(fragments[0])
        settings.frag2atoms = np.sort(fragments[1])
    elif morefrag:
        n_fragments = [x for x in n_fragments if x > 2]
        indices = [i for i, x in enumerate(n_fragments) if x ==
min(n_fragments)]
        counts = [list_of_fragments.count(list_of_fragments[x]) for x in
indices]
        fragments = list_of_fragments[indices[counts.index(max(counts))]]
        settings.fraglatoms = np.sort(fragments[0])
        settings.frag2atoms = np.sort([j for i in fragments[1:] for j in i])
        line_prependers(settings.logfile, "WARNING: more than two fragments
detected! Check fragments!\n\n")
    else:
        line_prependers(settings.logfile, "CRITICAL ERROR: couldn't determine
fragments automatically!\n\n")
        sys.exit("CRITICAL ERROR: couldn't determine fragments
automatically!")
    return settings
def get_single(file):
    structures.atoms = []
    structures.xyz = []
    structures.title = ['single structure']
    with open(file) as input_file:
        file_contents = input_file.read()
    if "Optimization completed." in file_contents:
        regex = r'\ -----
-----\n((?:(!\ -----
-----\n).)*)?\ -----
-----\n(?:(!\ -----
-----\n).)*)?Stationary\ point\ found'
        for match in re.finditer(regex, file_contents,
re.IGNORECASE|re.DOTALL):

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        raw_coordinates = match.group(1).strip().split("\n")
        break
    else:
        regex = r'\ -----
-----\n((?:?! \ -----
-----\n).*?)\ -----
-----\n(?:?! \ -----
-----\n).*?)Rotational\ constants'

        for match in re.finditer(regex, file_contents,
re.IGNORECASE|re.DOTALL):
            raw_coordinates = match.group(1).strip().split("\n")
            structures.xyz.append(np.array([x.split()[3:] for x in raw_coordinates]))
            structures.atoms = [x.split()[1] for x in raw_coordinates]
            structures.atoms = [periodic_table[int(x)] for x in structures.atoms]
            for i in range(len(structures.xyz)):
                structures.xyz[i] = structures.xyz[i].astype(float)
            return structures
def get_scan(file):
    with open(file) as input_file:
        file_contents = input_file.read()
        structures.xyz = []
        structures.atoms = []
        regex = r'-----
-----((?:?!-----
-----).*?)-----
---(?:?!-----
-).)*)?Stationary\ point\ found'

        for match in re.finditer(regex, file_contents, re.IGNORECASE|re.DOTALL):
            raw_coordinates = match.group(1).strip().split("\n")
            structures.xyz.append(np.array([x.split()[3:] for x in
raw_coordinates]))
            structures.atoms = [x.split()[1] for x in raw_coordinates]
            structures.atoms = [periodic_table[int(x)] for x in structures.atoms]
            for i in range(len(structures.xyz)):
                structures.xyz[i] = structures.xyz[i].astype(float)
            structures.title = [str(x) for x in range(len(structures.xyz))]
            return structures
def get_irc(file):
    with open(file) as input_file:
        file_contents = input_file.read()
        structures.xyz = []
        structures.atoms = []
        regex = r'Z\n -----
-----\n(.*?)\n -----
-----\n'

        for match in re.finditer(regex, file_contents, re.IGNORECASE|re.DOTALL):
            raw_coordinates = match.group(1).strip().split("\n")
            break
            structures.xyz.append(np.array([x.split()[3:] for x in raw_coordinates]))
            structures.atoms = [x.split()[1] for x in raw_coordinates]
            structures.atoms = [periodic_table[int(x)] for x in structures.atoms]
            regex = r'-----
-----((?:?!-----
-----).*?)-----
---(?:?!-----
-).)*)?Delta-x\ Convergence\ Met'

            for match in re.finditer(regex, file_contents, re.IGNORECASE|re.DOTALL):

```

```

        raw_coordinates = match.group(1).strip().split("\n")
        structures.xyz.append(np.array([x.split()[3:] for x in
raw_coordinates]))
    for i in range(len(structures.xyz)):
        structures.xyz[i] = structures.xyz[i].astype(float)
        structures.title = [str(x) for x in range(len(structures.xyz))]
    return structures
def check_fragments(settings, structures):
    for x in settings.fraglatoms:
        if int(x) > len(structures.atoms):
            line_prependers(settings.logfile, "CRITICAL ERROR: an atom number
in fragment 1 is higher than the highest atom number!\n\n")
            sys.exit("CRITICAL ERROR: an atom number in fragment 1 is higher
than the highest atom number!")
    for x in settings.frag2atoms:
        if int(x) > len(structures.atoms):
            line_prependers(settings.logfile, "CRITICAL ERROR: an atom number
in fragment 2 is higher than the highest atom number!\n\n")
            sys.exit("CRITICAL ERROR: an atom number in fragment 2 is higher
than the highest atom number!")
    if len(settings.fraglatoms) + len(settings.frag2atoms) !=
len(structures.atoms):
        line_prependers(settings.logfile, "CRITICAL ERROR: number of specified
fragment atoms does not equal total number of atoms!\n\n")
        sys.exit("CRITICAL ERROR: number of specified fragment atoms does not
equal total number of atoms!")
    if duplicates(settings.fraglatoms):
        line_prependers(settings.logfile, "CRITICAL ERROR: at least one atom
was defined more than once in fragment1!\n\n")
        sys.exit("CRITICAL ERROR: at least one atom was defined more than
once in fragment1!")
    if duplicates(settings.frag2atoms):
        line_prependers(settings.logfile, "CRITICAL ERROR: at least one atom
was defined more than once in fragment2!\n\n")
        sys.exit("CRITICAL ERROR: at least one atom was defined more than
once in fragment2!")
    elif len(set(settings.fraglatoms) & set(settings.frag2atoms)) > 0:
        line_prependers(settings.logfile, "CRITICAL ERROR: at least one atom
was defined in both fragments!\n\n")
        sys.exit("CRITICAL ERROR: at least one atom was defined in both
fragments!")
    return
def check_geo(structures, settings):
    natoms = len(structures.xyz[0])
    i = 0
    while i < len(settings.geo_dist):
        if len(settings.geo_dist[i]) != 2:
            del settings.geo_dist[i]
            line_prependers(settings.logfile, "WARNING: defined bond did not
have two elements! - This input is ignored\n\n")
        else:
            i = i+1
    i = 0
    while i < len(settings.geo_dist):
        if isInt(settings.geo_dist[i][0]) and isInt(settings.geo_dist[i][1]):
            i = i+1
        else:

```

```

        del settings.geo_dist[i]
        line_prepend(settings.logfile, "WARNING: defined bond did have
non-integer input! - This input is ignored\n\n")
    if len(settings.geo_dist) == 0:
        settings.geo_dist.append(getBonds(structures))
        line_prepend(settings.logfile, "WARNING: no correct definitions of
bonds found! - automatic detection of forming bonds\n\n")
    i = 0
    while i < len(settings.geo_dist):
        if int(settings.geo_dist[i][0]) > natoms or
int(settings.geo_dist[i][1]) > natoms or int(settings.geo_dist[i][0]) < 1 or
int(settings.geo_dist[i][1]) < 1 :
            del settings.geo_dist[i]
            line_prepend(settings.logfile, "WARNING: bond definition: atom
number out of range! - This input is ignored\n\n")
        else:
            i = i+1
    i=0
    while i < len(settings.geo_ang):
        if len(settings.geo_ang[i]) != 3:
            del settings.geo_ang[i]
            line_prepend(settings.logfile, "WARNING: defined angle did not
have three elements! - This input is ignored\n\n")
        else:
            i = i+1
    i = 0
    while i < len(settings.geo_ang):
        if isInt(settings.geo_ang[i][0]) and isInt(settings.geo_ang[i][1])
and isInt(settings.geo_ang[i][2]):
            i = i+1
        else:
            del settings.geo_ang[i]
            line_prepend(settings.logfile, "WARNING: defined angle did have
non-integer input! - This input is ignored\n\n")
    i=0
    while i < len(settings.geo_ang):
        if int(settings.geo_ang[i][0]) > natoms or
int(settings.geo_ang[i][1]) > natoms or int(settings.geo_ang[i][2]) > natoms
or int(settings.geo_ang[i][0]) < 1 or int(settings.geo_ang[i][1]) < 1 or
int(settings.geo_ang[i][2]) < 1:
            del settings.geo_ang[i]
            line_prepend(settings.logfile, "WARNING: angle definition: atom
number out of range! - This input is ignored\n\n")
        else:
            i = i+1
    i=0
    while i < len(settings.geo_dih):
        if len(settings.geo_dih[i]) != 4:
            del settings.geo_dih[i]
            line_prepend(settings.logfile, "WARNING: defined dihedral angle
did not have three elements! - This input is ignored\n\n")
        else:
            i = i+1
    i = 0
    while i < len(settings.geo_dih):
        if isInt(settings.geo_dih[i][0]) and isInt(settings.geo_dih[i][1])
and isInt(settings.geo_dih[i][2]) and isInt(settings.geo_dih[i][3]):

```



```

        i = i+1
    else:
        del settings.geo_dih[i]
        line_prependers(settings.logfile, "WARNING: defined dihedral angle
did have non-integer input! - This input is ignored\n\n")
    i=0
    while i < len(settings.geo_dih):
        if int(settings.geo_dih[i][0]) > natoms or
int(settings.geo_dih[i][1]) > natoms or int(settings.geo_dih[i][2]) > natoms
or int(settings.geo_dih[i][3]) > natoms or int(settings.geo_dih[i][0]) < 1 or
int(settings.geo_dih[i][1]) < 1 or int(settings.geo_dih[i][2]) < 1 or
int(settings.geo_dih[i][3]) < 1:
            del settings.geo_dih[i]
            line_prependers(settings.logfile, "WARNING: dihedral angle
definition: atom number out of range! - This input is ignored\n\n")
        else:
            i = i+1
    return settings
def structures_from_G(file, settings):
    file_object = open(file, 'r')
    input = (line for line in file_object)
    type = "single"
    for line in input:
        if "IRC-IRC-IRC" in line:
            type = "IRC"
            break
        elif "Scan" in line:
            type = "scan"
            break
    if type == "single":
        structures = get_single(file)
    elif type == "scan":
        structures = get_scan(file)
    else:
        structures = get_irc(file)
    file_object.seek(0)
    input_file = (line for line in file_object)
    for line in input_file:
        if "Charge =" in line:
            settings.charge = line.split()[2]
            settings.multi = line.split()[5]
            break
    return structures, settings
def structures_from_xyz(file):
    structures.atoms = []
    structures.xyz = []
    structures.title = []
    file_object = open(file, 'r')
    input = (line for line in file_object)
    for line in input:
        if isInt(line.strip()):
            n_atoms=int(line)
            break
    else:
        sys.exit('Error:\t\tNo xyz coordinates found in file: ' + file)
    structures.title.append(next(input).strip())
    for i in range(n_atoms):

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```

        l=next(input).split()
        if l[0] in periodic_table:
            structures.atoms.append(l[0])
        else:
            sys.exit('Error:\t\t something is wrong with the first structure
in file: '+file)
        coords=[float(x) for x in l[1:]]
        coords=np.array([coords])
        try:
            XYZ=np.concatenate((XYZ,coords), axis=0)
        except NameError:
            XYZ=coords
        structures.xyz.append(XYZ)
    del XYZ
    for line in input:
        try:
            if int(line.strip()) == n_atoms:
                structures.title.append(next(input).strip())
                for i in range(n_atoms):
                    l=next(input).split()
                    coords=[float(x) for x in l[1:]]
                    coords=np.array([coords])
                    try:
                        XYZ=np.concatenate((XYZ,coords), axis=0)
                    except NameError:
                        XYZ=coords
                    structures.xyz.append(XYZ)
                del XYZ
            except ValueError:
                pass
    return structures
def parse_in(input_filename, analysisonly):
    class settings:
        pass
    settings.void = []
    input_object = open(input_filename, 'r')
    input_object.seek(0)
    input_file = (line for line in input_object)
    for line in input_file:
        if len(line.split()) > 1:
            if line.split()[0].upper()+line.split()[1].upper() ==
"INPUTFILE":
                settings.ircfile = line.split()[-1]
                break
        else:
            sys.exit("No information on the structure input file could be
found!")
    input_object.seek(0)
    input_file = (line for line in input_object)
    settings.name = settings.ircfile
    for line in input_file:
        if len(line.split()) > 3:
            if line.split()[0].upper()+line.split()[1].upper() == "JOBNAME":
                try:
                    settings.name = line.split()[3]
                    break
                except IndexError:

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        break
    if analysisonly:
        settings.logfile= settings.name + "_analysisonly_log.txt"
        f= open(settings.logfile, 'w')
        f.close()
    else:
        settings.logfile= settings.name + "_log.txt"
        f= open(settings.logfile, 'w')
        f.close()
    try:
        structure_object = open(settings.ircfile, 'r')
    except FileNotFoundError:
        line_prependers(settings.logfile, "CRITICAL ERROR: structure input
file {0} not found!\n\n".format(settings.ircfile))
        sys.exit("CRITICAL ERROR: structure input file {0} not
found!".format(settings.ircfile))
        structure_object.seek(0)
        structure_file = (line for line in structure_object)
        settings.filetype="X"
        for line in structure_file:
            if "Gaussian, Inc." in line:
                settings.filetype="G"
                break
        if settings.filetype == "X":
            try:
                structures = structures_from_xyz(settings.ircfile)
            except StopIteration:
                line_prependers(settings.logfile, "CRITICAL ERROR: problem reading
structures from file {0}!\n\n".format(settings.ircfile))
                sys.exit("CRITICAL ERROR: problem reading structures from file
{0}!".format(settings.ircfile))
            else:
                structures, settings = structures_from_G(settings.ircfile, settings)
                input_object.seek(0)
                input_file = (line for line in input_object)
                try:
                    settings.charge
                except AttributeError:
                    settings.charge = 0
                for line in input_file:
                    if len(line.split()) > 0:
                        if line.split()[0].upper() == "CHARGE":
                            try:
                                settings.charge = int(line.split()[-1])
                                break
                            except IndexError:
                                break
                try:
                    settings.charge
                except AttributeError:
                    settings.charge = 0
                for line in input_file:
                    if len(line.split()) > 0:
                        if line.split()[0].upper() == "MULTIPLICITY":
                            try:
                                settings.charge = int(line.split()[-1])
                                break

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        except (IndexError, ValueError) as error:
            break
input_object.seek(0)
input_file = (line for line in input_object)
settings.fraglname = "fragment1"
for line in input_file:
    if len(line.split()) > 1:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT1NAME":
            try:
                settings.fraglname = line.split()[-1]
                break
            except (IndexError, ValueError) as error:
                break
input_object.seek(0)
input_file = (line for line in input_object)
settings.fraglcharge= 0
for line in input_file:
    if len(line.split()) > 1:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT1CHARGE":
            try:
                settings.fraglcharge = int(line.split()[-1])
                break
            except (IndexError, ValueError) as error:
                break
input_object.seek(0)
input_file = (line for line in input_object)
settings.fraglmulti = 1
for line in input_file:
    if len(line.split()) > 1:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT1MULTIPLICITY":
            try:
                settings.fraglmulti = int(line.split()[-1])
                break
            except (IndexError, ValueError) as error:
                break
input_object.seek(0)
input_file = (line for line in input_object)
settings.fraglenergy = 0
for line in input_file:
    if len(line.split()) > 1:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT1ENERGY":
            try:
                settings.fraglenergy = float(line.split()[-1])
                break
            except (IndexError, ValueError) as error:
                break
input_object.seek(0)
input_file = (line for line in input_object)
settings.fraglatoms = "auto"
for line in input_file:
    if len(re.split("\s+|,", line)) > 2:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT1ATOMS":

```

```

        try:
            settings.fraglatoms = re.split("\s+|,",line)[3:]
            break
        except IndexError:
            break
settings.fraglatoms = [int(x) for x in settings.fraglatoms if isInt(x)]
if len(settings.fraglatoms) == 0:
    settings.fraglatoms = "auto"
input_object.seek(0)
input_file = (line for line in input_object)
settings.frag2name = "fragment2"
for line in input_file:
    if len(line.split()) > 1:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT2NAME":
            try:
                settings.frag2name = line.split()[-1]
                break
            except IndexError:
                break
input_object.seek(0)
input_file = (line for line in input_object)
settings.frag2charge= 0
for line in input_file:
    if len(line.split()) > 1:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT2CHARGE":
            try:
                settings.frag2charge = int(line.split()[-1])
                break
            except (IndexError,ValueError) as error:
                break
input_object.seek(0)
input_file = (line for line in input_object)
settings.frag2multi = 1
for line in input_file:
    if len(line.split()) > 1:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT2MULTIPLICITY":
            try:
                settings.frag2multi = int(line.split()[-1])
                break
            except (IndexError,ValueError) as error:
                break
input_object.seek(0)
input_file = (line for line in input_object)
settings.frag2energy = 0
for line in input_file:
    if len(line.split()) > 1:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT2ENERGY":
            try:
                settings.frag2energy = float(line.split()[-1])
                break
            except (IndexError,ValueError) as error:
                break
input_object.seek(0)

```

```

input_file = (line for line in input_object)
settings.frag2atoms = "auto"
for line in input_file:
    if len(re.split("\s+|,",line)) > 2:
        if line.split()[0].upper()+line.split()[1].upper() ==
"FRAGMENT2ATOMS":
            try:
                settings.frag2atoms =re.split("\s+|,",line)[3:]
                break
            except IndexError:
                break
settings.frag2atoms = [int(x) for x in settings.frag2atoms if isInt(x)]
if len(settings.frag2atoms) == 0:
    settings.frag2atoms = "auto"
if settings.fraglatoms == "auto" and settings.frag2atoms == "auto":
    settings = auto_frag(structures,settings)
elif settings.fraglatoms == "auto":
    settings.fraglatoms = list(range(1,len(structures.atoms)+1))
    settings.fraglatoms = [item for item in settings.fraglatoms if item
not in set(settings.frag2atoms)]
elif settings.frag2atoms == "auto":
    settings.frag2atoms = list(range(1,len(structures.atoms)+1))
    settings.frag2atoms = [item for item in settings.frag2atoms if item
not in set(settings.fraglatoms)]
check_fragments(settings,structures)
structures.xyz_1 = []
settings.fraglatoms[:] = [x -1 for x in settings.fraglatoms]
for x in range(0, len(structures.xyz)):
    structures.xyz_1 = structures.xyz_1 +
[structures.xyz[x][settings.fraglatoms]]
structures.xyz_2 = []
settings.frag2atoms[:] = [x -1 for x in settings.frag2atoms]
for x in range(0, len(structures.xyz)):
    structures.xyz_2 = structures.xyz_2 +
[structures.xyz[x][settings.frag2atoms]]
structures.fraglatoms = []
for element in settings.fraglatoms:
    structures.fraglatoms = structures.fraglatoms +
[structures.atoms[element]]
structures.frag2atoms = []
for element in settings.frag2atoms:
    structures.frag2atoms = structures.frag2atoms +
[structures.atoms[element]]
input_object.seek(0)
input_file = (line for line in input_object)
settings.analysis = True
for line in input_file:
    if len(line.split()) > 0:
        if line.split()[0].upper() == "ANALYSIS":
            try:
                if line.split()[2].upper() == "YES":
                    settings.analysis = True
                    break
                elif line.split()[2].upper() == "NO":
                    settings.analysis = False
                    break
            except IndexError:

```

```

        break
    if settings.analysis:
        settings.geo_dist = [[]]
        with open(input_filename) as input_file:
            file_contents = input_file.read()
            for match in re.finditer(r'<distances>(.*?)</distances>',
file_contents, re.IGNORECASE|re.DOTALL):
                settings.geo_dist = match.group(1).strip().split('\n')
                settings.geo_dist = [element.split() for element in
settings.geo_dist]
                settings.geo_ang = []
                with open(input_filename) as input_file:
                    file_contents = input_file.read()
                    for match in re.finditer(r'<angles>(.*?)</angles>', file_contents,
re.IGNORECASE|re.DOTALL):
                        settings.geo_ang = match.group(1).strip().split('\n')
                        settings.geo_ang = [element.split() for element in
settings.geo_ang]
                        settings.geo_dih = []
                        with open(input_filename) as input_file:
                            file_contents = input_file.read()
                            for match in re.finditer(r'<dihedral>(.*?)</dihedral>',
file_contents, re.IGNORECASE|re.DOTALL):
                                settings.geo_dih = match.group(1).strip().split('\n')
                                settings.geo_dih = [element.split() for element in
settings.geo_dih]
                                if settings.geo_dist[0] == []:
                                    settings.geo_dist = [["auto"]]
                                for element in settings.geo_dist:
                                    if "auto" in element:
                                        auto_distances = getBonds(structures)
                                        settings.geo_dist = [ x for x in settings.geo_dist if "auto"
not in x]

                                        settings.geo_dist.append(auto_distances[0])
                                        settings.geo_dist.append(auto_distances[1])
                                        break
                                if len(settings.geo_ang)>0:
                                    if settings.geo_ang[0] == []:
                                        settings.geo_ang = []
                                if len(settings.geo_dih)>0:
                                    if settings.geo_dih[0] == "":
                                        settings.geo_dih = []
                                settings = check_geo(structures, settings)
                                input_object.seek(0)
                                input_file = (line for line in input_object)
                                settings.keepxyz = True
                                for line in input_file:
                                    if len(line.split()) > 2:
                                        if line.split()[0].upper()+line.split()[1].upper() == "KEEPXYZ":
                                            try:
                                                line.split()[3]
                                            except IndexError:
                                                settings.keepxyz = True
                                                break
                                        if line.split()[3].upper() == "YES":
                                            settings.keepxyz = True
                                        elif line.split()[3].upper() == "NO":

```



```

        settings.keepxyz = False
    else:
        settings.keepxyz = True
    break
input_object.seek(0)
input_file = (line for line in input_object)
settings.keepinput = True
for line in input_file:
    if len(line.split()) > 3:
        if
line.split()[0].upper()+line.split()[1].upper()+line.split()[2].upper() ==
"KEEPINPUTFILES":
    try:
        line.split()[4]
    except IndexError:
        settings.keepinput = True
        break
    if line.split()[4].upper() == "YES":
        settings.keepinput = True
    elif line.split()[4].upper() == "NO":
        settings.keepinput = False
    else:
        settings.keepinput = True
    break
input_object.seek(0)
input_file = (line for line in input_object)
settings.keepoutput = True
for line in input_file:
    if len(line.split()) > 3:
        if
line.split()[0].upper()+line.split()[1].upper()+line.split()[2].upper() ==
"KEEPOUTPUTFILES":
    try:
        line.split()[4]
    except IndexError:
        settings.keepoutput = True
        break
    if line.split()[4].upper() == "YES":
        settings.keepoutput = True
    elif line.split()[4].upper() == "NO":
        settings.keepoutput = False
    else:
        settings.keepoutput = True
    break
input_object.seek(0)
input_file = (line for line in input_object)
settings.keeplog = True
for line in input_file:
    if len(line.split()) > 3:
        if
line.split()[0].upper()+line.split()[1].upper()+line.split()[2].upper() ==
"KEEPLOGFILE":
    try:
        line.split()[4]
    except IndexError:
        settings.keeplog = True
        break

```

```

        if line.split()[4].upper() == "YES":
            settings.keeplog = True
        elif line.split()[4].upper() == "NO":
            settings.keeplog = False
        else:
            settings.keeplog = True
        break
input_object.seek(0)
input_file = (line for line in input_object)
settings.reorder = False
for line in input_file:
    if len(line.split()) > 2:
        if line.split()[0].upper() == "REORDER":
            try:
                line.split()[2]
            except IndexError:
                settings.reorder = False
                break
            if line.split()[2].upper() == "YES":
                settings.reorder = True
            elif line.split()[2].upper() == "NO":
                settings.reorder = False
            else:
                settings.reorder = False
            break
input_object.seek(0)
input_file = (line for line in input_object)
settings.reduce = False
for line in input_file:
    if len(line.split()) > 3:
        if line.split()[0].upper()+line.split()[1].upper() ==
"REDUCESTRUCTURES":
            try:
                line.split()[3]
            except IndexError:
                settings.reduce = False
                break
            if line.split()[3].upper() == "YES":
                settings.reduce = True
            elif line.split()[3].upper() == "NO":
                settings.reduce = False
            else:
                settings.reduce = False
            break
if settings.reduce:
    input_object.seek(0)
    input_file = (line for line in input_object)
    settings.reduce_tresh = 0.2
    for line in input_file:
        if len(line.split()) > 3:
            if line.split()[0].upper()+line.split()[1].upper() ==
"RMSDTRESHOLD":
                try:
                    line.split()[3]
                except IndexError:
                    settings.reduce_tresh = 0.2
                    break

```

```

        try:
            settings.reduce_tresh = float(line.split()[3].upper())
    )

    except ValueError:
        settings.reduce_tresh = 0.2
    break
input_object.seek(0)
input_file = (line for line in input_object)
settings.prepareonly = False
for line in input_file:
    if len(line.split()) > 3:
        if line.split()[0].upper()+line.split()[1].upper() ==
"PREPAREONLY":
            try:
                line.split()[3]
            except IndexError:
                settings.prepareonly = False
                break
            if line.split()[3].upper() == "YES":
                settings.prepareonly = True
            elif line.split()[3].upper() == "NO":
                settings.prepareonly = False
            else:
                settings.prepareonly = False
            break
input_object.seek(0)
input_file = (line for line in input_object)
settings.input_file_extension = "com"
for line in input_file:
    if len(line.split()) > 2:
        if
line.split()[0].upper()+line.split()[1].upper()+line.split()[2].upper() ==
"INPUTFILEEXTENSION":
            try:
                settings.input_file_extension = line.split()[4]
                break
            except IndexError:
                break
input_object.seek(0)
input_file = (line for line in input_object)
settings.output_file_extension = "log"
for line in input_file:
    if len(line.split()) > 2:
        if
line.split()[0].upper()+line.split()[1].upper()+line.split()[2].upper() ==
"OUTPUTFILEEXTENSION":
            try:
                settings.output_file_extension = line.split()[4]
                break
            except IndexError:
                break
settings.inputlayout = ""
with open(input_filename) as input_file:
    file_contents = input_file.read()
    for match in re.finditer(r'<layout>(.*?)</layout>', file_contents,
re.IGNORECASE|re.DOTALL):
        settings.inputlayout = match.group(1).strip()+'\n\n'

```

```
settings.submit_setting = ""
with open(input_filename) as input_file:
    file_contents = input_file.read()
    for match in re.finditer(r'<run_job>(.*?)</run_job>', file_contents,
re.IGNORECASE|re.DOTALL):
        settings.submit_setting = match.group(1).strip()
    return settings, structures
```

```

import numpy as np
def rotate(A, rot):
    B=np.dot(A, rot)
    return B
def procrustes(A, R):
    rot=find_rotation(A, R)
    B=rotate(A, rot)
    RMSD=calc_RMSD(B,R)
    return RMSD
def find_centroid(P):
    C=P.mean(axis=0)
    return C
def calc_RMSD(A, B):
    RMSD=0.0
    for i in range(3):
        for x in range(len(A)):
            RMSD += (A[x,i]-B[x,i])**2
    return np.sqrt(RMSD/len(A))
def find_rotation(A, R):
    C = np.dot(np.transpose(A), R)
    u, s, vh = np.linalg.svd(C)
    if (np.linalg.det(u) * np.linalg.det(vh)) < 0.0:
        s[-1] = -s[-1]
        u[:, -1] = -u[:, -1]
    rot = np.dot(u, vh)
    return rot
def center_xyz(structure, atoms, mode):
    if mode == 'c':
        V=-1*find_centroid(structure)
    elif mode == 'm':
        V=-1*find_centerofmass(structure, atoms)
    else:
        sys.exit('something went wrong')
    structure=structure+V
    return structure
def reorder(structures):
    if len(structures.xyz) == 1:
        return structures
    RMSD = []
    for i in range(0, len(structures.xyz)-1):
        RMSD = RMSD + [procrustes(structures.xyz[i],structures.xyz[i+1])]
    if np.amax(RMSD) > 3* np.mean(RMSD):
        cut = RMSD.index(np.amax(RMSD))
        rmsd1=procrustes(structures.xyz[0], structures.xyz[cut+1])
        rmsd2=procrustes(structures.xyz[cut], structures.xyz[cut+1])
        rmsd3=procrustes(structures.xyz[0], structures.xyz[-1])
        rmsd4=procrustes(structures.xyz[cut], structures.xyz[-1])
        if rmsd1 < rmsd2 and rmsd1 < rmsd3 and rmsd1 < rmsd4:
            structures.xyz = structures.xyz[cut::-1]+structures.xyz[cut+1:]
            structures.xyz_1 = structures.xyz_1[cut::-1]+structures.xyz_1[cut+1:]
            structures.xyz_2 = structures.xyz_2[cut::-1]+structures.xyz_2[cut+1:]
            structures.title = structures.title[cut::-1]+structures.title[cut+1:]

```

```

        elif rmsd2 < rmsd1 and rmsd2 < rmsd3 and rmsd2 < rmsd4:
            pass
        elif rmsd3 < rmsd1 and rmsd3 < rmsd2 and rmsd3 < rmsd4:
            structures.xyz = structures.xyz[cut::-1]+structures.xyz[:cut:-1]
            structures.xyz_1 = structures.xyz_1[cut::-1]+structures.xyz_1[:cut:-1]
            structures.xyz_2 = structures.xyz_2[cut::-1]+structures.xyz_2[:cut:-1]
            structures.title = structures.title[cut::-1]+structures.title[:cut:-1]
            elif rmsd4 < rmsd1 and rmsd4 < rmsd2 and rmsd4 < rmsd3:
                structures.xyz = structures.xyz[:cut+1]+structures.xyz[:cut:-1]
                structures.xyz_1 = structures.xyz_1[:cut+1]+structures.xyz_1[:cut:-1]
                structures.xyz_2 = structures.xyz_2[:cut+1]+structures.xyz_2[:cut:-1]
                structures.title = structures.title[:cut+1]+structures.title[:cut:-1]
            else:
                pass
        return structures
def reduce(structures, settings):
    if len(structures.xyz) == 1:
        return structures
    i=0
    count = 0
    while i < len(structures.xyz)-1:
        if procrustes(structures.xyz[i], structures.xyz[i+1]) >= settings.reduce_tresh:
            i = i+1
        else:
            count = count +1
            del structures.xyz[i+1]
            del structures.title[i+1]
            del structures.xyz_1[i+1]
            del structures.xyz_2[i+1]
    log = open(settings.logfile, 'a')
    log.write("Reduced structures by {0} ({1:.0f}%)!\n".format(count, float(count)/(len(structures.xyz)+count)*100))
    log.close()
    return structures

```

DIAS_analysis

```
radian2degree= 57.2958
hartree2kcal = 627.509
import numpy as np
import os, time
def getSCF(file):
    SCF = getmultiSCF(file)
    return SCF
def getmultiSCF(g09out):
    out = open(g09out, "r")
    SCFenergy = 0.00
    out.seek(0)
    out = reversed(list(out))
    for line in out:
        if "SCF Done" in line:
            SCFenergy = line.split()[4]
            break
        if "Energy=" in line:
            SCFenergy = line.split()[3]
            break
        elif "FINAL SINGLE POINT ENERGY" in line:
            SCFenergy = line.split()[4]
            break
        elif "Total energy in the final basis set" in line:
            SCFenergy = line.split()[8]
            break
        elif "Total DFT energy" in line:
            SCFenergy = line.split()[4]
            break
    try:
        SCFenergy = float(SCFenergy)
    except ValueError:
        SCFenergy = 0.00
    return SCFenergy
def getDistance(A, B):
    distance = np.sqrt( (A[0]-B[0])**2 + (A[1]-B[1])**2 + (A[2]-B[2])**2 )
    return distance
def getAngle(A, B, C):
    angle = 0.00
    BA_u = (A - B) / np.linalg.norm(A-B)
    BC_u = (C - B) / np.linalg.norm(C-B)
    angle = np.arccos(np.clip(np.dot(BA_u, BC_u), -1, 1))
    angle = angle * radian2degree
    return angle
def getDihedral(p0, p1, p2, p3):
    b0 = -1.0*(p1 - p0)
    b1 = p2 - p1
    b2 = p3 - p2
    b1 /= np.linalg.norm(b1)
    v = b0 - np.dot(b0, b1)*b1
    w = b2 - np.dot(b2, b1)*b1
    x = np.dot(v, w)
```

```

y = np.dot(np.cross(b1, v), w)
return np.degrees(np.arctan2(y, x))
def create_analysis_file(settings):
    analysis_file = open(settings.name+'_DIAS.txt', 'w')
    analysis_file.write('{0:<15}'.format('Step'))
    try:
        for x in range(0, len(settings.geo_dist)):
            analysis_file.write('{0:<18}'.format('Distance between'))
    except NameError:
        pass

    try:
        for x in range(0, len(settings.geo_ang)):
            analysis_file.write('{0:<18}'.format('Angle between'))
    except NameError:
        pass

    try:
        for x in range(0, len(settings.geo_dih)):
            analysis_file.write('{0:<18}'.format('Dihedral between'))
    except NameError:
        pass

    analysis_file.write('{0:<15}'.format('Total energy'))
    analysis_file.write('{0:<15}'.format('E(Int)'))
    analysis_file.write('{0:<15}'.format('E(Dist)'))
    analysis_file.write('{0:<15}'.format('E(Dist)'))
    analysis_file.write('{0:<15}'.format('E(Dist)'))
    analysis_file.write('{0:<20}'.format('E(SCF)'))
    analysis_file.write('{0:<20}'.format('E(SCF)'))
    analysis_file.write('{0:<20}'.format('E(SCF)'))
    analysis_file.write('\n')
    analysis_file.write('{0:<15}'.format(''))
    try:
        for x in range(0, len(settings.geo_dist)):
            analysis_file.write('{0:<18}'.format(str(settings.geo_dist[x][0])+'-'+
            str(settings.geo_dist[x][1])))
    except NameError:
        pass

    try:
        for x in range(0, len(settings.geo_ang)):
            analysis_file.write('{0:<18}'.format(settings.geo_ang[x][0]+'-'+
            settings.geo_ang[x][1]+'-'+ settings.geo_ang[x][2]))
    except NameError:
        pass

    try:
        for x in range(0, len(settings.geo_dih)):
            analysis_file.write('{0:<18}'.format(settings.geo_dih[x][0]+'-'+
            settings.geo_dih[x][1]+'-'+ settings.geo_dih[x][2]+'-'+
            settings.geo_dih[x][3]))
    except NameError:
        pass

    analysis_file.write('{0:<15}'.format(''))
    analysis_file.write('{0:<15}'.format(''))
    analysis_file.write('{0:<15}'.format('Total'))
    analysis_file.write('{0:<15}'.format(settings.frag1name))
    analysis_file.write('{0:<15}'.format(settings.frag2name))

```



```

analysis_file.write('{0:<20}'.format('complex'))
analysis_file.write('{0:<20}'.format(settings.frag1name))
analysis_file.write('{0:<20}'.format(settings.frag2name))
analysis_file.write('\n')
analysis_file.write('{0:<15}'.format(''))
try:
    for x in range(0, len(settings.geo_dist)):
        analysis_file.write('{0:<18}'.format('angstrom'))
except NameError:
    pass
try:
    for x in range(0, len(settings.geo_ang)):
        analysis_file.write('{0:<18}'.format('degree'))
except NameError:
    pass
try:
    for x in range(0, len(settings.geo_dih)):
        analysis_file.write('{0:<18}'.format('degree'))
except NameError:
    pass
analysis_file.write('{0:<15}'.format('kcal/mol'))
analysis_file.write('{0:<15}'.format('kcal/mol'))
analysis_file.write('{0:<15}'.format('kcal/mol'))
analysis_file.write('{0:<15}'.format('kcal/mol'))
analysis_file.write('{0:<15}'.format('kcal/mol'))
analysis_file.write('{0:<20}'.format('hartree'))
analysis_file.write('{0:<20}'.format('hartree'))
analysis_file.write('{0:<20}'.format('hartree'))
analysis_file.write('\n')
try:
    for x in range(0, len(settings.geo_dist)):
        analysis_file.write('{0:<18}'.format(''))
except NameError:
    pass
try:
    for x in range(0, len(settings.geo_ang)):
        analysis_file.write('{0:<18}'.format(''))
except NameError:
    pass
try:
    for x in range(0, len(settings.geo_dih)):
        analysis_file.write('{0:<18}'.format(''))
except NameError:
    pass
analysis_file.write('{0:<150}'.format(''))
analysis_file.write('\n')
analysis_file.close()
return
def analysis(settings, structures, x):
    analysis_file = open(settings.name+'_DIAS.txt', 'a')
    irc_SCF =
getSCF(settings.name+'_output/complex_{0:04d}'.format(x+1)+settings.output_f
ile_extension)
    fragment1_SCF =
getSCF(settings.name+'_output/'+settings.frag1name+'_{0:04d}'.format(x+1)+se
ttings.output_file_extension)

```

```

fragment2_SCF =
getSCF(settings.name+'_output/'+settings.frag2name+'_{0:04d}'.format(x+1))+se
ttings.output_file_extension)

fragment1_dist = fragment1_SCF - settings.frag1energy
fragment2_dist = fragment2_SCF - settings.frag2energy

interaction_energy = irc_SCF - (fragment1_SCF + fragment2_SCF)

distance_values = []
for y in range(0, len(settings.geo_dist)):
    distance_values = distance_values +
[getDistance(structures.xyz[x][int(settings.geo_dist[y][0])-
1],structures.xyz[x][int(settings.geo_dist[y][1])-1])]
    angle_values = []
    for y in range(0, len(settings.geo_ang)):
        angle_values = angle_values +
[getAngle(structures.xyz[x][int(settings.geo_ang[y][0])-
1],structures.xyz[x][int(settings.geo_ang[y][1])-
1],structures.xyz[x][int(settings.geo_ang[y][2])-1])]
    dihedral_values = []
    for y in range(0, len(settings.geo_dih)):
        dihedral_values = dihedral_values +
[getDihedral(structures.xyz[x][int(settings.geo_dih[y][0])-
1],structures.xyz[x][int(settings.geo_dih[y][1])-
1],structures.xyz[x][int(settings.geo_dih[y][2])-
1],structures.xyz[x][int(settings.geo_dih[y][3])-1])]

    analysis_file.write('{0:<15}'.format('{0:04d}'.format(x+1)))
    for element in distance_values:

analysis_file.write('{0:<18}'.format('{0:.5f}'.format(float(element))))
    for element in angle_values:

analysis_file.write('{0:<18}'.format('{0:.3f}'.format(float(element))))
    for element in dihedral_values:

analysis_file.write('{0:<18}'.format('{0:.3f}'.format(float(element))))
    analysis_file.write('{0:<15}'.format('{0:.5f}'.format(float((irc_SCF-
settings.frag1energy-settings.frag2energy)*hartree2kcal))))

analysis_file.write('{0:<15}'.format('{0:.5f}'.format(float(interaction_energ
y*hartree2kcal))))

analysis_file.write('{0:<15}'.format('{0:.5f}'.format(float((fragment1_dist+f
ragment2_dist)*hartree2kcal))))

analysis_file.write('{0:<15}'.format('{0:.5f}'.format(float(fragment1_dist*ha
rtree2kcal))))

analysis_file.write('{0:<15}'.format('{0:.5f}'.format(float(fragment2_dist*ha
rtree2kcal))))
    analysis_file.write('{0:<20}'.format('{0:.9f}'.format(float(irc_SCF))))

analysis_file.write('{0:<20}'.format('{0:.9f}'.format(float(fragment1_SCF))))

analysis_file.write('{0:<20}'.format('{0:.9f}'.format(float(fragment2_SCF))))

```

```

analysis_file.write('\n')
analysis_file.close()
def analysis_only(structures, settings):
    starttime= time.time()
    create_analysis_file(settings)
    for i in range(0, len(structures.xyz)):
        analysis(settings, structures, i)
    os.remove(settings.logfile)
    endtime=time.time()
    totaltime=str(endtime-starttime)
    seconds=totaltime.split('.')[0]
    milliseconds=float('0.'+totaltime.split('.')[1])*1000
    print('Analysis of {0} structures done in {1} seconds and {2:.0f}
ms'.format(len(structures.xyz),seconds, float(milliseconds)))
    return

```

Settings input file

The settings input file controls the actions taken by autoDIAS. In the following an example showing all available settings is presented. Settings are not case sensitive.

```
#-----  
Example input file  
#-----  
  
# relative or absolute path to file with structures. Can be xyz file or G09 output from IRC,  
Scan, single point, frequency or geometry opt calculation  
  
Input file = test.xyz  
  
# Define a job name. Default is the input file name without file extension  
  
Job name = test  
  
#-----  
Information on Structures  
#-----  
  
# Charge and multiplicity of the complex. Needs to be set for xyz files. Optional for G09 input  
  
charge = 0  
multiplicity = 1  
  
# Fragment information  
# fragment name, default is fragment1 or fragment2.  
Fragment1 name = Fragment1  
# fragment charge and multiplicity have to be provided. Default is charge 0 and multiplicity of 1  
Fragment1 charge = 0  
Fragment1 multiplicity = 1  
# list of the atoms in this fragment, provide a comma or space separated list, leave empty for  
automatic determination. If atom lists for both fragments are empty, then fragment 1 will contain  
the fragment containing atom 1  
Fragment1 atoms =  
# Electronic energy of this fragment, required for calculation of relative energy of the complex  
and distortion energies. Defaults to 0.  
Fragment1 energy = -243.485731  
  
Fragment2 name = Fragment2  
Fragment2 charge = 0  
Fragment2 multiplicity = 1  
Fragment2 atoms =  
Fragment2 energy = -464.752500  
  
#-----  
Information for Analysis  
#-----  
  
# Analysis can be turned on (YES) or off (NO), default is YES  
Analysis = YES  
  
# Distances can be extracted. Use atom numbers to define distances. Use one line per atom pair  
# write "auto" in line to attempt finding a total of two bonds that get formed or broken.  
<distances>  
1 2  
auto  
</distances>  
  
# Angles can be extracted. Use atom numbers to define angles. Use one line per angle  
<angles>  
1 2 3  
</angles>  
  
# Dihedral angles can be extracted. Use atom numbers to define angles. Use one line per angle  
<dihedral>  
1 2 3 4  
</dihedral>
```

```

#-----
Further Settings
#-----

# If set to YES autoDIA produces XYZ files of all complex and fragment structures and saves them
in a folder called <jobname>_xyz
Keep xyz = YES
# If set to YES autoDIA does not delete input files of all complex and fragment structures in
folder called <jobname>_input
Keep input files = YES
# If set to YES autoDIA does not delete output files of all complex and fragment structures in
folder called <jobname>_output
Keep output files = YES
# If set to YES autoDIA does not delete the log file called <jobname>_log.txt after successful
termination
Keep log file = YES

#Set if structures should be reordered
reorder = NO

#Eliminate very similar structures based on a certain RMSD threshold
Reduce structures = NO
RMSD threshold = 0.2

#Does only prepare input files but does not run them, does not do analysis (use -a flag for
analysis only)
Prepare only = NO

#-----
Input File Structure
#-----

# Input file structure for the chosen driver
# provide the settings for single point calculations
# use $filename and $coordinates $charge and $multiplicity in places where they are required
# Keep in mind the correct number of blank lines

<layout>
%mem=32GB
%nprocshared=16
# B3LYP/6-311+g(d,p) empiricaldispersion=gd3

Title

$charge $multiplicity
$coordinates

</layout>

#-----
Input File Structure
#-----

# provide the correct command to run the desired Software (e.g. Gaussian) on your system
# use $input and if needed $output for input and output file name

<run_job>
g09 $input $output
</run_job>

# Option to set the input file extension, some software might require a specific one. Defaults to
com
input file extension = com
# Option to set the output file extension, some software might require a specific one. Defaults
to log
output file extension = log

```

Log file

The log file contains information about the performed DIAS analysis. An example is shown here.

```
dsvatunek@Firefly
Sun Feb 17 02:18:46 2019
-----
Input file: SP.inp
Processed input and parsed structures in 0 seconds and 60 ms
-----
Determined settings and variables:

Job name                SP
Structure input          SP.log
Structure input filetype G

Analysis will be performed YES
  The following bond distances will be examined:

      Bond 1      atom 1: 1
                  atom 2: 28

      Bond 2      atom 1: 2
                  atom 2: 26

  The following angles will be examined:

      Angle 1      atom 1: 1
                  atom 2: 2
                  atom 3: 3

  The following dihedral angles will be examined:

      Dihedral 1   atom 1: 1
                  atom 2: 12
                  atom 3: 14
                  atom 4: 2

Keep xyz files          YES
Keep input files        YES
Keep output files       YES
Keep this log file      YES
Reorder structures      NO
Reduce structures       NO
Prepare input and exit  NO

Structure information

Input structure has 41 atoms with a molecular formula of:      C14H23N3O

Frag1 has 25 atoms with a molecular formula of:                C10H14O

Frag2 has 16 atoms with a molecular formula of:                 C4H9N3

Complex has a charge and multiplicity of: 0 1
Frag1 has a charge and multiplicity of: 0 1
Frag2 has a charge and multiplicity of: 0 1
Frag1 has an energy of: 0
Frag2 has an energy of: 0

-----
Produced input files for 1 structures in 0 seconds and 40 ms
-----
Sun Feb 17 02:18:46 2019      Starting      complex_0001      finished after 00:00:20.020667
Sun Feb 17 02:18:46 2019      Starting      Frag1_0001      finished after 00:00:00.020776
Sun Feb 17 02:18:46 2019      Starting      Frag2_0001      finished after 00:00:00.022710
-----
Sun Feb 17 02:18:46 2019 Finished after 00:00:00.244543
-----
```

DIAS file

The DIAS file named <jobname>_DIAS.txt contains all extracted information. The layout follows point numbers, geometric parameters, calculated energies and extracted energies. The exact layout depends on the number of geometric parameters. An example is shown here.

Step	Distance between 1-5 angstrom	Distance between 2-3 angstrom	Angle between 1-12-14 degree	Dihedral between 1-12-14-2 degree	Total energy kcal/mol	E(Int) kcal/mol	E(Dist) Total kcal/mol	E(Dist) Acrylaldehyde kcal/mol	E(Dist) Butadiene kcal/mol	E(SCF) complex hartree	E(SCF) Acrylaldehyde hartree	E(SCF) Butadiene hartree
0001	1.55363	1.54602	118.238	-2.967	-44.36679	-70.42620	25.62517	29.93003	16.33234	-347.794051036	-191.804308649	-155.873511011
0002	1.55427	1.54597	118.198	-2.954	-44.71007	-70.42620	29.86722	11.07337	18.79385	-347.793906081	-191.801471451	-155.873588072
0003	1.55488	1.54593	118.170	-2.948	-44.60533	-79.34802	34.74269	13.14050	21.60219	-347.793739169	-191.798177261	-155.869112691
0004	1.55548	1.54590	118.132	-2.960	-44.48615	-84.68224	40.19609	15.47349	24.72260	-347.793549241	-191.794459411	-155.864139993
0005	1.55602	1.54588	118.086	-2.992	-44.36833	-89.74912	45.38079	17.70106	27.67973	-347.793361487	-191.790909538	-155.859427513
0006	1.55658	1.54585	118.024	-3.043	-44.23596	-95.12297	50.88701	20.06604	30.82096	-347.793150550	-191.787140701	-155.854421631
0007	1.55718	1.54580	117.946	-3.109	-44.09071	-100.74364	56.65293	22.53197	34.12096	-347.792919077	-191.783211001	-155.849162743
0008	1.55784	1.54571	117.848	-3.187	-43.93351	-106.55337	62.61987	25.06326	37.55661	-347.792668552	-191.779177130	-155.843687685
0009	1.55860	1.54555	117.729	-3.283	-43.76145	-112.49197	68.73051	27.62639	41.10412	-347.792394369	-191.775092505	-155.838034371
0010	1.55956	1.54526	117.581	-3.417	-43.56816	-118.49208	74.92392	30.18818	44.73574	-347.792086339	-191.771010037	-155.832247014
0011	1.56062	1.54487	117.422	-3.592	-43.37916	-123.62797	80.24881	32.35765	47.89116	-347.791785149	-191.767552768	-155.827218518
0012	1.56204	1.54430	117.218	-3.849	-43.16141	-128.70472	85.54331	34.48167	51.06165	-347.791438130	-191.764167927	-155.822166021
0013	1.56406	1.54302	116.952	-4.198	-42.90630	-133.67237	90.76607	36.54252	54.22355	-347.791031593	-191.760883739	-155.817127215
0014	1.56672	1.54360	116.671	-4.551	-42.65757	-137.69413	95.03656	38.20149	56.83506	-347.790635220	-191.758240000	-155.812965493
0015	1.57141	1.54264	116.336	-4.937	-42.36679	-141.58096	99.21417	39.80183	59.41234	-347.790171829	-191.755689696	-155.808858334
0016	1.58006	1.54270	115.978	-5.305	-42.01638	-145.30330	103.28692	41.34104	61.94587	-347.789613417	-191.753236803	-155.804820894
0017	1.59434	1.54340	115.662	-5.582	-41.56938	-148.81868	107.24930	42.81966	64.42963	-347.788901078	-191.750880473	-155.800862767
0018	1.61813	1.54497	115.410	-5.747	-40.83641	-152.69403	111.85762	44.51829	67.33933	-347.787733005	-191.748173533	-155.796225861
0019	1.64649	1.54708	115.292	-5.760	-39.83849	-156.15015	116.31166	46.14065	70.17102	-347.786142719	-191.745588145	-155.791713282
0020	1.67735	1.54957	115.272	-5.672	-38.56933	-159.18998	120.62065	47.69552	72.92513	-347.784120181	-191.743110295	-155.787324316
0021	1.71515	1.55288	115.334	-5.486	-36.77912	-162.25584	125.47673	49.43467	76.04206	-347.781267296	-191.740388760	-155.782357174
0022	1.75408	1.55665	115.460	-5.240	-34.71197	-164.87259	130.16662	51.10307	79.05755	-347.777973088	-191.737793088	-155.777551687
0023	1.79372	1.56097	115.634	-4.953	-32.42853	-167.10861	134.68007	52.70639	81.97368	-347.774334192	-191.735124954	-155.772904523
0024	1.83380	1.56596	115.844	-4.635	-29.98584	-169.02293	139.03709	54.24596	84.79113	-347.770441506	-191.732671492	-155.768414629
0025	1.87418	1.57175	116.086	-4.295	-27.43637	-170.66208	143.22572	55.71801	87.50771	-347.766378664	-191.730325638	-155.764085478
0026	1.91469	1.57855	116.353	-3.939	-24.82578	-172.05653	147.23075	57.11206	90.11869	-347.762218433	-191.728104068	-155.759924622
0027	1.96100	1.58786	116.687	-3.520	-21.81388	-173.35675	151.54287	58.58557	92.95729	-347.757418657	-191.725755874	-155.755401011
0028	2.00708	1.59924	117.047	-3.100	-18.80807	-174.28966	155.48159	59.88217	95.59942	-347.752628587	-191.723696611	-155.751190514
0029	2.05264	1.61320	117.427	-2.692	-15.83190	-174.70055	158.86865	60.91467	97.95398	-347.747885757	-191.722044223	-155.747438278
0030	2.09728	1.63026	117.822	-2.313	-12.89745	-174.32019	161.42274	61.58132	99.84142	-347.743209417	-191.720981847	-155.744430456
0031	2.14054	1.65086	118.223	-1.983	-10.01013	-173.04287	163.03274	61.94531	101.08743	-347.738608170	-191.720401786	-155.742444803
0032	2.18193	1.67523	118.622	-1.717	-7.17565	-171.40704	164.23140	62.30553	101.92586	-347.734091129	-191.719827740	-155.741108673
0033	2.22107	1.70330	119.010	-1.527	-4.40317	-169.82887	165.42570	62.72169	102.70400	-347.729672903	-191.719164545	-155.739868628
0034	2.25779	1.73468	119.382	-1.417	-1.71279	-168.36282	166.65004	63.12712	103.52291	-347.725385499	-191.718518451	-155.738563612
0035	2.29212	1.76885	119.733	-1.384	0.86075	-166.99703	167.85779	63.49413	104.36365	-347.721284300	-191.717933583	-155.737223804
0036	2.32424	1.80526	120.062	-1.423	3.27182	-165.72088	168.99270	63.82744	105.16526	-347.717442023	-191.717402419	-155.735946370
0037	2.35444	1.84341	120.370	-1.525	5.46762	-164.55522	170.02284	64.13833	105.88451	-347.713942788	-191.716906989	-155.734800164
0038	2.38302	1.88286	120.659	-1.684	7.39388	-163.54791	170.94179	64.43657	106.50522	-347.710873086	-191.716431707	-155.733811005
0039	2.41035	1.92324	120.932	-1.892	9.99881	-162.76286	171.76168	64.73205	107.02963	-347.708315467	-191.715960832	-155.732975306
0040	2.43684	1.96423	121.193	-2.137	10.23880	-162.26343	172.50223	65.03312	107.46911	-347.706339426	-191.715481049	-155.732274947
0041	2.46294	2.00551	121.448	-2.407	11.09272	-162.09294	173.18566	65.34599	107.83967	-347.704978607	-191.714982461	-155.731684415
0042	2.49238	2.05197	121.735	-2.723	11.60794	-162.30076	173.90870	65.71585	108.13285	-347.704157562	-191.714393043	-155.731121594
0043	2.51580	2.08770	121.956	-2.960	11.72056	-162.72922	174.44979	66.01668	108.43310	-347.703978078	-191.713913641	-155.730738719
0044	2.51914	2.09283	121.988	-2.996	11.71866	-13.41642	25.13507	9.08899	16.04608	-347.703981116	-191.804633757	-155.877966922
0045	2.54915	2.13892	122.291	-3.325	11.52880	-9.61069	21.13949	7.44822	13.69127	-347.704283668	-191.807248493	-155.881719554
0046	2.57985	2.18448	122.590	-3.649	11.08584	-6.75434	17.84019	6.11148	11.72871	-347.704989570	-191.809378735	-155.884847097
0047	2.60723	2.22473	122.853	-3.951	10.53877	-4.87009	15.40886	5.14204	10.26682	-347.705861384	-191.810923629	-155.887176772
0048	2.63446	2.26488	123.111	-4.273	9.88820	-3.49054	13.37874	4.34581	9.03292	-347.706898142	-191.812192500	-155.889143112
0049	2.66131	2.30503	123.362	-4.619	9.16278	-2.52698	11.68976	3.69559	7.99417	-347.708054171	-191.813228700	-155.890798467
0050	2.68763	2.34524	123.606	-4.990	8.38789	-1.90584	10.29373	3.17028	7.12345	-347.709289044	-191.814065828	-155.892186058
0051	2.71342	2.38545	123.844	-5.380	7.58962	-1.56337	9.15299	2.75374	6.39925	-347.710561159	-191.814729631	-155.893340136
0052	2.73879	2.42549	124.077	-5.781	6.79283	-1.44105	8.23388	2.43129	5.80259	-347.711830923	-191.815243488	-155.894290972
0053	2.76076	2.46024	124.277	-6.134	6.11244	-1.47260	7.58504	2.21427	5.37077	-347.712915205	-191.815589338	-155.894979127
0054	2.78268	2.49461	124.472	-6.485	5.45708	-1.60005	7.05713	2.04648	5.01065	-347.713959577	-191.815856732	-155.895553008
0055	2.80463	2.52853	124.661	-6.831	4.83251	-1.79582	6.62833	1.91711	4.71122	-347.714954900	-191.816062892	-155.896030191
0056	2.82664	2.56202	124.842	-7.174	4.24329	-2.03621	6.27950	1.81664	4.46285	-347.715893880	-191.816222991	-155.896425983
0057	2.84871	2.59508	125.012	-7.512	3.69316	-2.30203	5.95919	1.73778	4.25741	-347.716770571	-191.816348672	-155.896753384
0058	2.87085	2.62772	125.169	-7.845	3.18415	-2.57904	5.76319	1.67513	4.08806	-347.717581724	-191.816448510	-155.897023257
0059	2.88986	2.65536	125.292	-8.125	2.78122	-2.81731	5.59853	1.63127	3.96726	-347.718223842	-191.816518399	-155.897215769
0060	2.90892	2.68268	125.405	-8.400	2.40924	-3.05085	5.46009	1.59454	3.86555	-347.718816632	-191.816576936	-155.897377852
0061	2.92803	2.70965	125.506	-8.671	2.06771	-3.27589	5.34630	1.56381	3.78009	-347.719360986	-191.816626385	-155.897514036
0062	2.94719	2.73625	125.595	-8.944	1.75588	-3.48966	5.24585	1.53715	3.70839	-347.719857824	-191.816668390	-155.897638830
0063	2.96637	2.76248	125.669	-9.226	1.47302	-3.68987	5.16290	1.51457	3.64832	-347.720308584	-191.816704371	-155.897724021
0064	2.98549	2.78841	125.731	-9.526	1.21743	-3.87555	5.09298	1.49505	3.59792	-347.720715902	-191.816735477	-155.897804338
0065	3.00445	2.81412	125.779	-9.854	0.98625	-4.04678	5.03302	1.47804	3.55498	-347.721084314	-191.816762592	-155.897872770
0066	3.02313	2.83973	125.814	-10.214	0.77682	-4.20365	4.98048	1.46314	3.51734	-347.721418056	-191.816786340	-155.897932761
0067	3.04145	2.86529	125.839	-10.611	0.58713	-4.34654	4.93367	1.45021	3.48346	-347.721720350	-191.816806939	-155.897986747
0068	3.05939	2.89076	125.858	-11.019	0.41904	-4.49074	4.89438	1.43910	3.45221	-347.721993481</		

Plotting

Results of autoDIAS can be read by the numpy genfromtxt or the Excel data from text function. In the following a commented script of how to plot resulting data using Python 3.7.1 and Matplotlib are presented.

Plotting of total, distortion and interaction energies for a single geometric parameter (used for Figure 5)

```
#example of plotting a complete DIAS analysis along an IRC as shown in Figure 5
import numpy as np
from matplotlib import pyplot as plt
import matplotlib.patches as mpatches

#create plot
f= plt.figure(figsize=(2.5, 2.5),dpi=300)
ax1 = f.add_subplot(1,1,1)

#read data from autoDIA output
a = np.genfromtxt('IRC1_DIA.txt',skip_header=4)

#set axis
ax1.set_ylabel('Energy')
ax1.set_xlabel('Forming bond distance')
ax1.axis([np.amax(a[:,2])+0.1, np.amin(a[:,2])-0.1, np.amin(a[:,6])-20, np.amax(a[:,7])+20])
ax1.axhline(y=0, color='grey', linestyle='--',linewidth = 0.5)

#the second geometric parameter (column 3 - keep in mind that Numpy counting starts at 0)
representing a bond length is used as X-Value
x = a[:,2]
#In this case column 7 contains information about interaction energy
y = a[:,6]
ax1.plot(x,y,'-',color='g',linewidth = 1)
#In this case column 8 contains information about total distortion energy
y = a[:,7]
ax1.plot(x,y,'-',color='r',linewidth = 1)
#In this case column 9 contains information about the acrolein distortion energy
y = a[:,8]
ax1.plot(x,y,'-',color='lightcoral',linewidth = 0.5)
#In this case column 10 contains information about the butadiene distortion energy
y = a[:,9]
ax1.plot(x,y,'-',color='orange',linewidth = 0.5)
#In this case column 6 contains information about the total energy. Plotted last to be on top.
y = a[:,5]
ax1.plot(x,y,'-',color='k',linewidth = 1)

#creating the legend
black_patch = mpatches.Patch(color='k', label='Total energy')
red_patch = mpatches.Patch(color='r', label='Distortion energy')
green_patch = mpatches.Patch(color='g', label='Interaction energy')
coral_patch = mpatches.Patch(color='lightcoral', label='Acrolein distortion energy')
orange_patch = mpatches.Patch(color='orange', label='Butadiene distortion energy')
plt.legend(handles=[black_patch,red_patch,coral_patch,orange_patch,green_patch],prop={'size':
5},loc=3,frameon=False)

ax_limits=[2.75, 1.75, -50, 50]
ax1.axis(ax_limits)

f.tight_layout()
f.savefig('IRC.png')
```


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Other files

autoDIAS-1.0.1.zip (22.28 KiB)

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